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FILE COVERS 1907 - 15 May 2003 VOL 138 ISS 20  
 FILE LAST UPDATED: 14 May 2003 (20030514/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 121; d que 119; d que 125; d que 132; d que 139; d que 156

L3	219941	SEA FILE=HCAPLUS ABB=ON	OXIDATION+OLD, NT/CT
L4	72723	SEA FILE=HCAPLUS ABB=ON	OXIDATION CATALYSTS+NT/CT
L5	60005	SEA FILE=HCAPLUS ABB=ON	METALLOPORPHYRINS+OLD, NT/CT
L17	1054	SEA FILE=HCAPLUS ABB=ON	L5 (L)CAT/RL -Role CAT = catalyst
L18	511	SEA FILE=HCAPLUS ABB=ON	L17 AND (L3 OR L4)
L20	13065	SEA FILE=HCAPLUS ABB=ON	APROTIC
L21	4	SEA FILE=HCAPLUS ABB=ON	L18 AND L20

L4 and L5 L17

L3	219941	SEA FILE=HCAPLUS ABB=ON	OXIDATION+OLD, NT/CT
L4	72723	SEA FILE=HCAPLUS ABB=ON	OXIDATION CATALYSTS+NT/CT
L5	60005	SEA FILE=HCAPLUS ABB=ON	METALLOPORPHYRINS+OLD, NT/CT
L6	1	SEA FILE=REGISTRY ABB=ON	75-89-8
L7	1	SEA FILE=REGISTRY ABB=ON	920-66-1
L8	34	SEA FILE=REGISTRY ABB=ON	(536-80-1/BI OR 75-89-8/BI OR 920-66-1/BI OR 1088-11-5/BI OR 1119-94-4/BI OR 127256-73-9/BI OR 13002-65-8/BI OR 1515-14-6/BI OR 179024-48-7/BI OR 20927-53- 1/BI OR 245329-97-9/BI OR 288-32-4/BI OR 2888-64-4/BI OR 363608-72-4/BI OR 363608-73-5/BI OR 363608-74-6/BI OR 363608-75 -7/BI OR 363608-76-8/BI OR 363608-77-9/BI OR 364043-33-4/BI OR 371-62-0/BI OR 375-01-9/BI OR 422-05-9/BI OR 439-14-5/BI OR 4797-43-7/BI OR 604-75-1/BI OR 631-61-8/BI OR 7722-84-1/BI OR 79968-43-7/BI OR 846-50-4/BI OR 91463-17-1/BI OR 937-14-4/BI OR 963-39-3/BI OR 98-08-8/BI)
L9	9	SEA FILE=REGISTRY ABB=ON	L8 AND F/ELS
L10	1	SEA FILE=REGISTRY ABB=ON	C4H4F6O/MF AND L9
L12	1	SEA FILE=REGISTRY ABB=ON	L9 AND BENZENE
L13	3273	SEA FILE=HCAPLUS ABB=ON	L6
L14	1286	SEA FILE=HCAPLUS ABB=ON	L7
L15	92	SEA FILE=HCAPLUS ABB=ON	L10
L16	1212	SEA FILE=HCAPLUS ABB=ON	L12
L17	1054	SEA FILE=HCAPLUS ABB=ON	L5 (L)CAT/RL
L18	511	SEA FILE=HCAPLUS ABB=ON	L17 AND (L3 OR L4)
L19	1	SEA FILE=HCAPLUS ABB=ON	(L13 OR L14 OR L15 OR L16) AND L18

Oxidation Catal  
 and  
 metallo (L)

Cat  
 Role

L3 219941 SEA FILE=HCAPLUS ABB=ON OXIDATION+OLD, NT/CT  
 L4 72723 SEA FILE=HCAPLUS ABB=ON OXIDATION CATALYSTS+NT/CT  
 L5 60005 SEA FILE=HCAPLUS ABB=ON METALLOPORPHYRINS+OLD, NT/CT  
 L17 1054 SEA FILE=HCAPLUS ABB=ON L5(L)CAT/RL  
 L18 511 SEA FILE=HCAPLUS ABB=ON L17 AND (L3 OR L4)  
 L23 8464 SEA FILE=HCAPLUS ABB=ON PHASE TRANSFER CATALYSTS+OLD, RTCS/CT  
 L25 4 SEA FILE=HCAPLUS ABB=ON L18 AND L23

L3 219941 SEA FILE=HCAPLUS ABB=ON OXIDATION+OLD, NT/CT  
 L4 72723 SEA FILE=HCAPLUS ABB=ON OXIDATION CATALYSTS+NT/CT  
 L5 60005 SEA FILE=HCAPLUS ABB=ON METALLOPORPHYRINS+OLD, NT/CT  
 L17 1054 SEA FILE=HCAPLUS ABB=ON L5(L)CAT/RL  
 L18 511 SEA FILE=HCAPLUS ABB=ON L17 AND (L3 OR L4)  
 L26 1 SEA FILE=REGISTRY ABB=ON DICHLOROMETHANE/CN  
 L27 1 SEA FILE=REGISTRY ABB=ON DICHLOROETHANE/CN  
 L28 3 SEA FILE=REGISTRY ABB=ON TRICHLOROETHANE/CN  
 L29 31418 SEA FILE=HCAPLUS ABB=ON (L26 OR L27 OR L28)  
 L30 507 SEA FILE=HCAPLUS ABB=ON L18 NOT L29  
 L31 36649 SEA FILE=HCAPLUS ABB=ON SOLVENTS/CT  
 L32 3 SEA FILE=HCAPLUS ABB=ON L30 AND L31

L5 60005 SEA FILE=HCAPLUS ABB=ON METALLOPORPHYRINS+OLD, NT/CT  
 L17 1054 SEA FILE=HCAPLUS ABB=ON L5(L)CAT/RL  
 L26 1 SEA FILE=REGISTRY ABB=ON DICHLOROMETHANE/CN  
 L27 1 SEA FILE=REGISTRY ABB=ON DICHLOROETHANE/CN  
 L28 3 SEA FILE=REGISTRY ABB=ON TRICHLOROETHANE/CN  
 L29 31418 SEA FILE=HCAPLUS ABB=ON (L26 OR L27 OR L28)  
 L37 5128 SEA FILE=HCAPLUS ABB=ON (OXIDATION# OR OXIDN#)/OBI(1W)ORG?  
 L39 5 SEA FILE=HCAPLUS ABB=ON L17 AND L37 NOT L29

L3 219941 SEA FILE=HCAPLUS ABB=ON OXIDATION+OLD, NT/CT  
 L4 72723 SEA FILE=HCAPLUS ABB=ON OXIDATION CATALYSTS+NT/CT  
 L5 60005 SEA FILE=HCAPLUS ABB=ON METALLOPORPHYRINS+OLD, NT/CT  
 L17 1054 SEA FILE=HCAPLUS ABB=ON L5(L)CAT/RL  
 L26 1 SEA FILE=REGISTRY ABB=ON DICHLOROMETHANE/CN  
 L27 1 SEA FILE=REGISTRY ABB=ON DICHLOROETHANE/CN  
 L28 3 SEA FILE=REGISTRY ABB=ON TRICHLOROETHANE/CN  
 L29 31418 SEA FILE=HCAPLUS ABB=ON (L26 OR L27 OR L28)  
 L52 12593 SEA FILE=HCAPLUS ABB=ON HYDROCARBONS, REACTIONS/CT  
 L53 2765 SEA FILE=HCAPLUS ABB=ON L52(L)OXID?  
 L56 23 SEA FILE=HCAPLUS ABB=ON L17 AND (L3 OR L4) AND L53 NOT L29

=> s 121 or 119 or 125 or 132 or 139 or 156

L57 35 L21 OR L19 OR L25 OR L32 OR L39 OR L56

=> fil uspatf; d que 148

FILE 'USPATFULL' ENTERED AT 11:35:45 ON 15 MAY 2003  
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 13 May 2003 (20030513/PD)  
 FILE LAST UPDATED: 13 May 2003 (20030513/ED)  
 HIGHEST GRANTED PATENT NUMBER: US6564383  
 HIGHEST APPLICATION PUBLICATION NUMBER: US2003088899

CA INDEXING IS CURRENT THROUGH 13 May 2003 (20030513/UPCA)  
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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2003  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2003

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
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>>> publications, starting in 2001, for the inventions covered in <<<  
>>> USPATFULL. A USPATFULL record contains not only the original <<<  
>>> published document but also a list of any subsequent <<<  
>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
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>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

L45 97 SEA FILE=USPATFULL ABB=ON METALLOPORPHYRINS/CT  
L46 12 SEA FILE=USPATFULL ABB=ON CATALY?/IT (L)L45  
L47 682015 SEA FILE=USPATFULL ABB=ON OXID? OR OXID?/IT  
L48 12 SEA FILE=USPATFULL ABB=ON L46 AND L47

=> dup rem 157,148  
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PROCESSING COMPLETED FOR L57  
PROCESSING COMPLETED FOR L48  
L58 47 DUP REM L57 L48 (0 DUPLICATES REMOVED)  
ANSWERS '1-35' FROM FILE HCAPLUS  
ANSWERS '36-47' FROM FILE USPATFULL

=> d ibib ab hitrn 1-47

L58 ANSWER 1 OF 47 HCAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2003:336636 HCAPLUS  
DOCUMENT NUMBER: 138:309859  
TITLE: Catalytic oxidations using ruthenium porphyrins  
AUTHOR(S): Ezhova, Maria B.; James, Brian R.  
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.  
SOURCE: Catalysis by Metal Complexes (2003), 26(Advances in Catalytic Activation of Dioxygen by Metal Complexes), 1-77  
PUBLISHER: CODEN: CMCOES; ISSN: 0920-4652  
Kluwer Academic Publishers



DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review; the major goal of the Chapter is to review developments in the use of Ru-porphyrin complexes as homogeneous (or matrix-supported) catalysts for oxygenation and oxidn. processes. The subject was given impetus with the discovery of a remarkable reaction in which a Ru(II) porphyrin complex reacted with O<sub>2</sub> to give a trans-dioxo-Ru(VI) species. Such species, which can be formed from a wide range of O-atom donors, were shown subsequently to be capable of acting as a bis(monoxygenase) in transferring both the coordinated oxo ligands (as O-atoms) to olefinic substrates, satd. hydrocarbons, phosphines, and thioethers, and the processes become catalytic in the presence of excess of the O-atom donor. Further, the dioxo species can also exhibit oxidase-like activity, and effect stoichiometric or catalytic oxidative-dehydrogenation of phenols, alkoxyarenes, alcs., and amines. Use of chiral porphyrins has led to catalytic, asym. epoxidn. and hydroxylations, even though radical intermediates are invoked, as well as oxygenation of racemic substrates (phosphines and more interestingly tertiary alkanes) to yield chiral products by kinetic resoln. processes. The reaction mechanisms invoked range from genuine O-atom transfer (from RuVI, RuV, or RuIV species, where the disproportionation reaction [2 O=RuIV .dblharw. RuII + O=RuVI=O] is important), to free-radical induced processes, particularly when the porphyrin ligands are extensively halogenated, as Ru complexes generally of such porphyrins are extremely active in radical-type decompr. of hydroperoxides, often present as trace impurities in hydrocarbon substrates.

REFERENCE COUNT: 281 THERE ARE 281 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 2 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:123801 HCAPLUS

DOCUMENT NUMBER: 136:294443

TITLE: CO<sub>2</sub>-Expanded Solvents: Unique and Versatile Media for Performing Homogeneous Catalytic Oxidations

AUTHOR(S): Wei, Ming; Musie, Ghezai T.; Busch, Daryle H.; Subramaniam, Bala

CORPORATE SOURCE: Department of Chemical and Petroleum Engineering and Department of Chemistry, University of Kansas, Lawrence, KS, 66045-2223, USA

SOURCE: Journal of the American Chemical Society (2002), 124 (11), 2513-2517

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The work summarized here demonstrates a new concept for exploiting dense phase CO<sub>2</sub>, media considered to be green solvents, for homogeneous catalytic oxidn. reactions. According to this concept, the conventional org. solvent medium used in catalytic chem. reactions is replaced substantially (up to 80 vol.%) by CO<sub>2</sub>, at moderate pressures (tens of bars), to create a continuum of CO<sub>2</sub>-expanded solvent media. A particular benefit is found for oxidn. catalysis; the presence of CO<sub>2</sub> in the mixed medium increases the O<sub>2</sub> solv. by .apprx.100 times compared to that in the neat org. solvent while the retained org. solvent serves an essential role by solubilizing the transition metal catalyst. CO<sub>2</sub>-expanded solvents provide optimal properties for maximizing oxidn. rates that are typically 1-2 orders of magnitude greater than those obtained with either the neat org. solvent or supercrit. CO<sub>2</sub> as the reaction medium. These advantages are demonstrated with examples of homogeneous oxidns. of a substituted phenol and of cyclohexene by mol. O<sub>2</sub> using transition metal catalysts, Co Schiff-base and Fe porphyrin complexes, resp., in CO<sub>2</sub>-expanded CH<sub>3</sub>CN.

IT 16456-81-8

RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 (CO<sub>2</sub>-expanded solvents as unique and versatile media for performing homogeneous catalytic oxidns.)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 3 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:675277 HCAPLUS

DOCUMENT NUMBER: 138:153305

TITLE: Remarkable solvent effect on the yield and specificity of oxidation of naphthalene catalyzed by iron(III) porphyrins

AUTHOR(S): Khavasi, Hamid Reza; Hosseiny Davarani, S. Saeed; Safari, Nasser

CORPORATE SOURCE: Chemistry Department, Shahid Beheshti University, Evin, Tehran, 19839, Iran

SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 188(1-2), 115-122

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:153305

AB Oxidn. of naphthalene was performed with tetrakis(pentafluorophenyl)porphyrin iron(III) chloride (F<sub>20</sub>TPPFe<sub>4</sub>Cl<sub>4</sub>) or tetrakis(2,6-dichlorophenyl)porphyrin iron(III) chloride (TDCPPFe<sub>4</sub>Cl<sub>4</sub>) or tetramesitylporphyrin iron(III) chloride (TMPFe<sub>4</sub>Cl<sub>4</sub>) as catalyst and m-chloroperbenzoic acid or pentafluoriodosylbenzene or tert-Bu hydroperoxide as oxidant in different media in the presence of imidazole as cocatalyst. In an aprotic solvent (CH<sub>3</sub>CN:CH<sub>2</sub>Cl<sub>2</sub> 1:1) and in the presence of F<sub>20</sub>TPPFe<sub>4</sub>Cl<sub>4</sub>, 1-naphthol, 2-naphthol and 1,4-naphthoquinone yields based on m-chloroperbenzoic acid oxidant were 77.7, 2.1 and 5.6%, resp. The best yield for 1,4-naphthoquinone occurred in methanol with F<sub>20</sub>TPPFe<sub>4</sub>Cl<sub>4</sub> and was 52.8%. The effect of bases on the yield and specificity of the naphthalene oxidn. were studied. When imidazole was changed to pyridine in F<sub>20</sub>TPPFe<sub>4</sub>Cl<sub>4</sub>, the yield of 1-naphthol decreased from 77.7 to 55.3%, whereas for TDCPPFe<sub>4</sub>Cl<sub>4</sub> catalyst, the yield changed from 61.1 to 18.3%.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 4 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:218837 HCAPLUS

DOCUMENT NUMBER: 137:5840

TITLE: Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons

AUTHOR(S): Avdeev, M. V.; Bagrii, E. I.; Maravin, G. B.; Korolev, Yu. M.

CORPORATE SOURCE: Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, 117912, Russia

SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2002), 43(1), 38-44

CODEN: KICAA8; ISSN: 0023-1584

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Conference proceedings. The oxidn. of cyclic hydrocarbons by potassium peroxymonosulfate catalyzed by the iron and manganese complexes of tetra-(4-N-butylpyridinium)porphyrin, tetraphenylporphyrin, and mixed porphyrins contg. Ph and butylpyridyl substituents was studied in an aq. acetonitrile medium. The test catalysts were dissolved in the reaction

medium or adsorbed on layered aluminosilicates. It was found that the immobilization of metal complexes on layered aluminosilicates, as well as the bromination of porphyrins, decreased the activity of catalysts in a no. of cases, although it improved their stability. The addn. of pyridine in an equimolar amt. with respect to metal complexes to the reaction mixt. increased the activity of dissolved manganese complexes. An increase in the no. of butylpyridyl meso-substituents in a porphyrin mol. improved the catalytic activity of a metal complex.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 5 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:115086 HCPLUS

DOCUMENT NUMBER: 134:178573

TITLE: Process for the metalloporphyrin catalyzed oxidation of organic compounds

INVENTOR(S): Bernardelli, Patrick

PATENT ASSIGNEE(S): Warner Lambert Company, USA

SOURCE: PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809
PRIORITY APPLN. INFO.:			US 1999-148079P	P 19990810
			US 1999-150101P	P 19990820
			WO 2000-EP7726	W 20000809

OTHER SOURCE(S): CASREACT 134:178573

AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, **aprotic**, polyhalogenated solvent (benzotrifluoride). Oxidn. of diazepam is conducted to mimic oxidn. (metab.) in biol. systems. The products of the oxidn. of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert **aprotic** solvent shows improved oxidn. yields when compared to prior art (e.g., CH<sub>3</sub>CN-CH<sub>2</sub>C<sub>12</sub>-water mixts.).

IT 920-66-1, 1,1,1,3,3,3-Hexafluoro-2-propanol

RL: CAT (Catalyst use); USES (Uses)

(co-solvent; process for metalloporphyrin-catalyzed **oxidn.** of org. compds.)

IT 75-89-8, 2,2,2-Trifluoroethanol

RL: NUU (Other use, unclassified); USES (Uses)

(co-solvent; process for metallocporphyrin-catalyzed **oxidn.** of  
org. compds.)

IT 98-08-8, Benzotrifluoride

RL: NUU (Other use, unclassified); USES (Uses)  
(process for metallocporphyrin-catalyzed **oxidn.** of org  
compds.)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 6 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:694140 HCAPLUS

DOCUMENT NUMBER: 136:166904

TITLE: Iron polynitroporphyrins bearing up to eight  
.beta.-nitro groups as interesting new catalysts for  
H<sub>2</sub>O<sub>2</sub>-dependent hydrocarbon oxidation: unusual  
regioselectivity in hydroxylation of alkoxybenzenes

AUTHOR(S): Bartoli, Jean-Francois; Le Barch, Karine; Palacio,  
Magali; Battioni, Pierrette; Mansuy, Daniel  
CORPORATE SOURCE: UMR 8601, Universite Paris V, Paris, 75270, Fr.  
SOURCE: Chemical Communications (Cambridge, United Kingdom)  
(2001), (18), 1718-1719

CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of iron porphyrins bearing one to eight .beta.-nitro substituents  
were synthesized and evaluated as catalysts for hydrocarbon oxidn. with  
H<sub>2</sub>O<sub>2</sub>. Iron porphyrins bearing five or six .beta.-nitro groups were the  
best catalysts for cyclooctene epoxidn. and adamantine or anisole  
hydroxylation without need of a cocatalyst. Very different  
regioselectivities were obsd. with either H<sub>2</sub>O<sub>2</sub> or PhIO as oxidants, as  
shown by an unusual ortho-hydroxylation of alkoxybenzenes highly favored  
in the H<sub>2</sub>O<sub>2</sub>-dependent oxidns.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 7 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:344513 HCAPLUS

DOCUMENT NUMBER: 134:326198

TITLE: Catalytic oxidation of alkanes or cycloalkanes using  
metallocporphyrins

INVENTOR(S): Guo, Cancheng; Liu, Qiang; Zhang, Xiaobing

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhanli Shengqing Gongkai Shuomingshu, 8 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1269343	A	20001011	CN 2000-113225	20000117
PRIORITY APPLN. INFO.:	CN 2000-113225 20000117			
OTHER SOURCE(S):	CASREACT 134:326198; MARPAT 134:326198			
AB	Alkanes or cycloalkanes are oxidized at 1 atm air at 25-120.degree. in the presence of 40-200 ppm metallocporphyrin catalyst and catalyst adjuvant. The mole ratio of metallocporphyrin to catalyst adjuvant is 1:3-5. The metallocporphyrin or its oxide is [5,10,15,20-tetra(4- R1-3-R2-2-R3- phenyl)porphyrin]MX or [5,10,15,20-tetra(4-R1- 3-R2-2-R3- phenyl)porphyrin]M1 [5,10,15,20-tetra(4-R1-3- R2-2-R3-phenyl)porphyrin]M2 oxide (M, M1, and/or M2 = transition metal or lanthanide; and R1, R2, and/or R3 = H, alkyl, alkoxy, halo, amino, alkylamino, glycosyl, or			

cyclodextrin group; and X = acetate, acetoacetonato, halide, or other acid group-type anion). The carrier for metalloporphyrin catalyst is silica gel, mol. sieve, Al2O3, zeolite, sepiolite, porous ceramics, polyvinyl chloride, polyvinyl perchloride, or polystyrene, etc. The catalyst adjuvant is salt or oxide of Cu, Zn, Fe, Co, Mn, Cr, or Ni, etc.

L58 ANSWER 8 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2000:442953 HCPLUS  
DOCUMENT NUMBER: 133:176887  
TITLE: Evidence for the Participation of Two Distinct Reactive Intermediates in Iron(III) Porphyrin Complex-Catalyzed Epoxidation Reactions  
AUTHOR(S): Nam, Wonwoo; Lim, Mi Hee; Lee, Ha Jin; Kim, Cheal  
CORPORATE SOURCE: Department of Chemistry and Division of Molecular Life Sciences, Ewha Womans University, Seoul, 120-750, S. Korea  
SOURCE: Journal of the American Chemical Society (2000), 122(28), 6641-6647  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB We have studied the competitive epoxidns. of olefins with cis- and trans-stilbenes and with cyclooctene and trans-stilbene in iron-porphyrin complex-catalyzed epoxidn. reactions by H2O2, tert-Bu hydroperoxide (t-BuOOH), and m-chloroperoxybenzoic acid (m-CPBA) in protic solvent (i.e., a solvent mixt. of CH3OH and CH2Cl2) and aprotic solvent (i.e., a solvent mixt. of CH3CN and CH2Cl2) at room temp. under catalytic reaction conditions. The competitive epoxidns. were also carried out with in situ generated high-valent iron(IV) oxo porphyrin cation radical complexes in aprotic solvent under stoichiometric reaction conditions. By detg. the ratios of epoxide products formed in the competitive epoxidns., we were able to conclude unambiguously that the reactive species generated in protic solvent are high-valent iron(IV) oxo porphyrin cation radical complexes 3 [FeIV:O-Porp.bul.+] and the intermediates formed in aprotic solvent are oxidant-iron porphyrin intermediates 2 [e.g., FeIIIOOH-Porp]. A protic solvent such as methanol is proposed to function as a general-acid catalyst, thereby increasing the rate of O-O bond cleavage of 2 to form 3. In the absence of general-acid catalysis such as in aprotic solvent, the rate of O-O bond cleavage of 2 is relatively slow and 2 transfers its oxygen to olefins prior to the formation of 3. To further examine the effect of the general-acid catalysis on the nature of epoxidizing intermediates, we carried out competitive epoxidns. in the solvent mixts. of alc./CH2Cl2 using alcs. of varying pKa values and in the presence of an acid (i.e., HClO4) in aprotic solvent. The product ratios were found to vary depending on the strength of the solvent acidity, demonstrating that the reaction of 2 with olefin competes with the O-O bond cleavage of 2 that leads to the formation of 3. We also reported for the first time that a high-valent iron(IV) oxo porphyrin cation radical intermediate contg. electron-deficient porphyrin ligand shows an unexpected preference for trans-stilbene over cis-stilbene in the competitive epoxidns. of cis- and trans-stilbenes..

REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 9 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2000:735661 HCPLUS  
DOCUMENT NUMBER: 134:91666  
TITLE: Metalloporphyrin catalytic oxidations of hydrocarbons by H2O2  
AUTHOR(S): Rocha Gonsalves, Antonio M. d'A.; Serra, Armenio C.  
CORPORATE SOURCE: Departamento de Quimica, Universidade de Coimbra,

SOURCE: Coimbra, P-3049, Port.  
Journal of Porphyrins and Phthalocyanines (2000),  
4(6), 598-603  
CODEN: JPPHFZ; ISSN: 1088-4246  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The metalloporphyrin catalytic oxidn. of hydrocarbons using dil. hydrogen peroxide as oxygen donor with a two-phase system in the presence of an excess of benzoic acid is studied. Porphyrins derived from meso-tetrakis(2,6-dichlorophenyl)porphyrin and bearing sulfonamide substituents at .beta. or meso positions and halogens at .beta. positions were used. The system allowed for very efficient catalytic epoxidns. and hydroxylations of hydrocarbons. It is proved that the excess of benzoic acid is crit. to the catalyst efficiency and stability. The role of the lipophilic acid in this system is discussed.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 10 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2000:273368 HCPLUS  
DOCUMENT NUMBER: 133:22890  
TITLE: Synthesis and characterization of zeolite-encapsulated metalloporphyrins  
AUTHOR(S): Nakagaki, S.; Xavier, C. R.; Wosniak, A. J.; Mangrich, A. S.; Wypych, F.; Cantao, M. P.; Denicolo, I.; Kubota, L. T.  
CORPORATE SOURCE: Departamento de Quimica, Universidade Federal do Parana, Curitiba, Brazil  
SOURCE: Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2000), 168(3), 261-276  
CODEN: CPEAEH; ISSN: 0927-7757  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Metalloporphyrins of FeIII and CuII were prep'd. inside the large pores of the zeolite NaY by a process of sequential introduction of components followed by assembly inside the void space of the zeolite. The appropriate process chosen for the porphyrin synthesis was using the propionic acid solvent for reaction between pyrrole and benzaldehyde and this solvent was not destructive for zeolite. The powder X-ray diffraction data confirmed that the crystallinity of the zeolite was maintained. The resulting materials were purified by Soxhlet extractor. The zeolite-included metalloporphyrins were identified for studies using UV-Vis, FTIR and EPR Spectroscopy, CA (chem. anal.), AAS (at. absorption spectroscopy), TG/DSC, XRD, SEM and 13C-NMR techniques. The catalytic activity of these products was examd. and the catalyst showed to be a promising catalytic system to aliph. hydrocarbon oxidn. reactions.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 11 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2000:179461 HCPLUS  
DOCUMENT NUMBER: 132:278747  
TITLE: Study on catalytic activation of dioxygen by polymer quasi-porphyrin complexes  
AUTHOR(S): Wang, Rong-Min; Wang, Yun-Pu; Lei, Zi-Qiang  
CORPORATE SOURCE: Chemistry & Chemical Engineering College, Northwest Normal University, Lanzhou, 730070, Peop. Rep. China  
SOURCE: Xibei Shifan Daxue Xuebao, Ziran Kexueban (2000), 36(1), 100-103  
CODEN: XDXKEH; ISSN: 1001-988X  
PUBLISHER: Xibei Shifan Daxue

DOCUMENT TYPE: Journal; General Review  
LANGUAGE: Chinese

AB A review with 21 refs. The development of efficient catalysts for the selective oxidn. of hydrocarbons in presence of mol. oxygen under mild condition has remained a difficult challenge. Much attention has been paid to the construction. of the active center - the quasi-porphyrin complex - and its polymer surroundings for mimicing the structure and properties of enzyme. We have used polymer-supported porphyrin and Schiff base complexes. They show higher activitites in oxidn. of alkylbenzene, cyclohexene and long-chain linear aliph. olefins.

L58 ANSWER 12 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:445418 HCPLUS

DOCUMENT NUMBER: 131:144244

TITLE: Catalysis of hydrocarbon oxidation by polyhalogenated ruthenium porphyrins and studies on the origins of enantioselectivity in metallocporphyrin catalyzed olefin epoxidations

AUTHOR(S): Shalyaev, Kirill V.

CORPORATE SOURCE: Princeton Univ., Princeton, NJ, USA

SOURCE: (1998) 201 pp. Avail.: UMI, Order No. DA9920463

From: Diss. Abstr. Int., B 1999, 60(2), 643

DOCUMENT TYPE: Dissertation

LANGUAGE: English

AB Unavailable

L58 ANSWER 13 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:93389 HCPLUS

DOCUMENT NUMBER: 128:180083

TITLE: Rapid catalytic oxygenation of hydrocarbons with perhalogenated ruthenium porphyrin complexes

AUTHOR(S): Groves, John T.; Shalyaev, Kirill V.; Bonchio, Marcella; Carofiglio, Tommaso

CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA

SOURCE: Studies in Surface Science and Catalysis (1997), 110(3rd World Congress on Oxidation Catalysis, 1997), 865-872

CODEN: SSCTDM; ISSN: 0167-2991

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Conference proceedings. Perhalogenated ruthenium porphyrins were found to be efficient catalysts for the oxygenation of hydrocarbons including secondary alkanes and benzene in the presence of 2,6-dichloropyridine N-oxide under mild conditions in **aprotic** media. Up to 15,000 turnovers and rates of 800 TO/min were obtained. A mechanism where Ru(III) - Ru(V) intermediates play an important role is proposed and discussed.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 14 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:386113 HCPLUS

DOCUMENT NUMBER: 127:105856

TITLE: Biomimetic **oxidation** of organic substrates by chemical models of cytochrome P-450 and related heme monooxygenases

AUTHOR(S): Chauhan, S. M. S.

CORPORATE SOURCE: Department of Chemistry, University of Delhi, Delhi, 110 007, India

SOURCE: Journal of the Indian Chemical Society (1996), 73(12), 637-645

PUBLISHER: Indian Chemical Society  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English  
 AB A review with 72 refs. Cytochromes P 450 are membrane-bound heme monooxygenases that catalyze the monooxygenation of a wide range of org. substrates by utilization of dioxygen and NADPH or NADH as reducing agents. The development of chem. models for cytochromes P 450 has been initiated to understand the mol. mechanisms of different cytochromes P 450 and to develop suitable catalysts for selective and mild oxidn. in org. synthesis and oxidative metab. of drugs, agrochems., and xenobiotics. The synthesis of metalloporphyrins and chem. models for cytochrome P 450 and demonstration of their biomimetic activities in oxidizing org. substrates is examd.

L58 ANSWER 15 OF 47 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1996:680698 HCPLUS  
 DOCUMENT NUMBER: 126:59546  
 TITLE: Aerobic oxidation of hydrocarbons catalyzed by electronegative iron salen complexes  
 AUTHOR(S): Boettcher, Arnd; Grinstaff, Mark W.; Labinger, Jay A.; Gray, Harry B.  
 CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA  
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 191-200  
 CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A no. of salen derivs. bearing electroneg. substituents and their corresponding iron(III) chloro complexes have been prepd. Several of the complexes catalyze aerobic oxidn. of cyclohexene, primarily to allylic oxidn. products. Evidence supports a radical chain autoxidn. mechanism, with the complex functioning to decomp. intermediate alkyl hydroperoxides. Activity is obsd. only for complexes with relatively high Fe(III/II) redn. potentials, but the incomplete correlation of activity with potential indicates that more subtle structural and electronic effects also play an important role in dtg. the rates of the catalytic reactions.

IT 16456-81-8  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 (aerobic oxidn. of hydrocarbons catalyzed by electroneg. iron salen complexes)

L58 ANSWER 16 OF 47 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1996:680700 HCPLUS  
 DOCUMENT NUMBER: 126:103763  
 TITLE: Nonradical tetrabutylammonium monopersulfate oxidation of hydrocarbons catalyzed by  $[\text{Mn}304\text{bipy}_4(\text{H}_2\text{O})_2](\text{ClO}_4)_4$   
 AUTHOR(S): Wessel, Jeremy; Crabtree, Robert H.  
 CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven, CT, 06520, USA  
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 13-22  
 CODEN: JMCCF2; ISSN: 1381-1169  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 126:103763  
 AB Tetrabutylammonium monopersulfate ( $2\text{NBu}_4\text{HSO}_5 \cdot \text{cntdot} \cdot \text{NBu}_4\text{HSO}_4 \cdot \text{cntdot} \cdot (\text{NBu}_4)_2\text{SO}_4$ ) is an effective primary oxidant with a high tendency to promote oxo

transfer rather than radical pathways in catalysis. Nonradical hydrocarbon oxidn. is seen with the complex  $[\text{Mn}3\text{O}4\text{bipy}_4(\text{H}_2\text{O})_2](\text{ClO}_4)_4$  as catalyst as indicated by mechanistic studies; this contrasts with the radical pathways found for the same catalyst with t-BuOOH as the primary oxidant. The catalyst is robust, giving up to 15000 catalytic turnovers, and very efficient, the rate of 1-alkene epoxidn. being 4000 turnovers/h.

L58 ANSWER 17 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1996:103134 HCPLUS  
DOCUMENT NUMBER: 124:218485  
TITLE: The mechanism of catalytic hydrocarbon oxidation by molecular oxygen and halogenated ruthenium and iron porphyrins  
AUTHOR(S): Birnbaum, Eva Rachel  
CORPORATE SOURCE: California Institute of Technology, Pasadena, CA, USA  
SOURCE: (1995) 355 pp. Avail.: Univ. Microfilms Int., Order No. DA9601103  
From: Diss. Abstr. Int., B 1995, 56(9), 4876  
DOCUMENT TYPE: Dissertation  
LANGUAGE: English  
AB Unavailable

L58 ANSWER 18 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1995:502796 HCPLUS  
DOCUMENT NUMBER: 123:82524  
TITLE: The highly efficient oxidation of olefins, alcohols, sulfides and alkanes with heteroaromatic N-oxides catalyzed by ruthenium porphyrins  
AUTHOR(S): Otake, Hiro; Higuchi, Tsunehiko; Hirobe, Masaaki  
CORPORATE SOURCE: Faculty Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan  
SOURCE: Heterocycles (1995), 40(2), 867-903  
CODEN: HTCYAM; ISSN: 0385-5414  
PUBLISHER: Japan Institute of Heterocyclic Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 123:82524  
AB The O atom transfer reactions from 2,6-disubstituted pyridine N-oxides to olefins, allyl or benzyl alcs. and sulfides were efficiently catalyzed by Ru porphyrins, and these substrates were converted into epoxides, aldehydes and sulfoxides, resp., with high selectivity. These oxidns. also proceeded using other heteroarom. N-oxides, such as pyrazine N-oxides, as oxidants. The catalytic activity of Ru porphyrin complexes was enhanced by the addn. of a small amt. of HCl or HBr. In the presence of these acids, the oxidns. of alkanes or aliph. alcs. with 2,6-dichloropyridine N-oxides were also efficiently catalyzed by Ru porphyrin complexes, and alcs. or ketones were afforded as oxidn. products with high selectivity. In the hydroxylation of adamantane, Ru porphyrins work very efficiently as catalysts, giving a turnover no. of up to 120,000. This system offers practical advantages, such as mild conditions, tractability of oxidants and easy overall procedures. In the case of the reactions with HCl or HBr, one possibility in the reaction mechanism is that the activity of Ru porphyrins is enhanced in part by the coordination of Cl- or Br- as axial ligands.

IT 14172-90-8

RL: CAT (Catalyst use); USES (Uses)  
(lack of catalysis in oxidn. of olefins and alcs. and alkanes and sulfides by heteroarom. N-oxides)

L58 ANSWER 19 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1995:952970 HCPLUS  
DOCUMENT NUMBER: 124:67840  
TITLE: Synthesis and catalytic performance of polymer-supported metallocporphyrins bearing polyglycol

AUTHOR(S): chains  
Yu, Xiaoqi; Wei, Tingxian; Lan, Zhongwei; You,  
Jingsong; Zhao, Huaming  
CORPORATE SOURCE: Dep. Chem., Sichuan Univ., Chengdu, 610064, Peop. Rep.  
China  
SOURCE: Fenzi Cuihua (1995), 9(4), 244-50  
CODEN: FECUEN; ISSN: 1001-3555  
PUBLISHER: Zhongguo Kexueyuan Lanzhou Huaxue Wuli Yanjiuso  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese

AB Synthesis and catalytic performance of polymer-supported metalloporphyrins bearing polyglycol chains in CH<sub>2</sub>C<sub>12</sub>/H<sub>2</sub>O two-phase system were studied. The influence of pH values, concn. of NaOCl, axial ligands and phase transfer catalysts on the epoxidn. of styrene catalyzed by those catalysts have also been investigated. The exptl. results show that manganese (III) porphyrins bound to chloromethylated polystyrene which bears some polyglycerol chains are efficient catalysts for the epoxidn. of styrene by sodium hypochloride. The introduction of polyglycol chain increases the amt. of oxidant in the org. phase by extg. -OCl from the aq. phase. Under these conditions, the anion -OCl assocd. with the polyglycol chain is extremely reactive as an oxidant. In all factors studied exptl., the influence of pH values in aq. soln. is the greatest.

L58 ANSWER 20 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1995:286499 HCPLUS  
DOCUMENT NUMBER: 122:94975  
TITLE: Oxidation reactions of Mononuclear Manganese(III) Complexes  
AUTHOR(S): Gangopadhyay, Sumana; Ali, Mahammad; Banerjee, Pradyot  
CORPORATE SOURCE: Department of Inorganic Chemistry, Indian Association  
for the Cultivation of Science, Calcutta, 700 032,  
India  
SOURCE: Coordination Chemistry Reviews (1994), 135/136,  
399-427  
CODEN: CCHRAM; ISSN: 0010-8545  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review, with 73 refs., is given on the oxidn. reactions of various Mn(III) coordinated mols. The reactions are categorized primarily with respect to the type of Mn(III) complexes. Emphasis is given to the reactivity of the Mn(III) complexes derived from aminopolycarboxylic acids, acetylacetone, porphyrins, bipyridine, and pyrophosphoric acid with various org., inorg., and biochem. electron donors. Kinetic and mechanistic features assocd. with the interactions are highlighted and analyzed critically. The utility and scope of the catalytic oxidn. of hydrocarbons and secondary amines by Mn(III) porphyrins are discussed at length.

L58 ANSWER 21 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1995:535380 HCPLUS  
DOCUMENT NUMBER: 123:32378  
TITLE: Metalloporphyrin-catalyzed oxidation of hydrocarbons with dioxygen  
AUTHOR(S): Mlodnicka, Teresa  
CORPORATE SOURCE: Institute Catalysis and Surface Chemistry, Polish  
Academy Sciences, Krakow, Pol.  
SOURCE: Metalloporphyrins Catal. Oxid. (1994), 261-96.  
Editor(s): Sheldon, Roger A. Dekker: New York, N. Y.  
CODEN: 60SIAM  
DOCUMENT TYPE: Conference; General Review  
LANGUAGE: English  
AB A review with 154 refs.

L58 ANSWER 22 OF 47 HCAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1994:76659 HCAPLUS  
DOCUMENT NUMBER: 120:76659  
TITLE: Catalytic oxidation of saturated and aromatic hydrocarbons by tert-butyl hydroperoxide in the presence of rare earth porphyrin complexes  
AUTHOR(S): Vedernikov, A. N.; Kochnev, D. O.; Suslov, D. A.; Solomonov, B. N.  
CORPORATE SOURCE: Kazan. Gos. Univ., Russia  
SOURCE: Doklady Akademii Nauk (1993), 330(2), 200-3 [Chem.]  
CODEN: DAKNEQ; ISSN: 0869-5652  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
OTHER SOURCE(S): CASREACT 120:76659  
AB Oxidn. of hydrocarbons, such as cyclohexane, adamantane, and PhMe, by Me<sub>3</sub>COOH in C<sub>6</sub>H<sub>6</sub> catalyzed by 15 title complexes was studied. The overall yield of products is linearly dependent on catalyst concn. in the oxidn. of hydrocarbons catalyzed by (meso-tetraphenylporphyrinato)lutetium(III) hydroxide. The porphyrin ligand is an essential part of the catalyst.

L58 ANSWER 23 OF 47 HCAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1992:650744 HCAPLUS  
DOCUMENT NUMBER: 117:250744  
TITLE: Selective oxygenation of hydrocarbons and sulfoxidation of thioethers by dioxygen with a Mn-porphyrin-based cytochrome P450 model system using zinc as electron donor  
AUTHOR(S): Lu, W. Y.; Bartoli, J. F.; Battioni, P.; Mansuy, D.  
CORPORATE SOURCE: Lab. Chim. Biochem. Pharmacol. Toxicol., Univ. Paris V, Paris, 75270, Fr.  
SOURCE: New Journal of Chemistry (1992), 16(5), 621-8  
CODEN: NJCHE5; ISSN: 0398-9836  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 117:250744  
AB Cyclooctene epoxidn. by O<sub>2</sub> occurs, with consumption of reducing equivs. from Zn and protons from acetic acid, in the presence of two catalysts, Mn(TPP)Cl (H<sub>2</sub>TPP = 5,10,15,20-tetraphenylporphyrin) and 1-methylimidazole (1-MeIm). A comparative study made on ten different Mn(III) or Fe(III) porphyrin catalysts, ten nitrogen base cocatalysts and various carboxylic acids showed that the most efficient system involves Mn(TPP)Cl, 1-MeIm and CH<sub>3</sub>COOH in addn. to O<sub>2</sub> and Zn in a CH<sub>3</sub>CN:CH<sub>2</sub>Cl<sub>2</sub> mixt. This system selectively epoxidizes 2-methylhept-2-ene, cyclohexene, (+)-limonene, cis-stilbene and .alpha.-ionone with yields based on Zn between 34 and 58% and rates between 1 and 3 turnovers per min. It also epoxidizes 1-nonene, a less reactive alkene, and oxidizes alkanes like cyclooctane, cyclohexane, adamantane, indan, tetralin and heptane to the corresponding alcs. and ketones, but with lower yields (between 1 and 36%). Thioethers are selectively oxidized to the corresponding sulfoxides with yields up to 68%. The system exhibits a stereochem. for cis- and trans-stilbene epoxidn., a regioselectivity for the oxidn. of cyclohexene, limonene and heptane, and a chemoselectivity for the oxidn. of a cyclooctene-cyclooctane mixt., almost identical to those of the Mn(TPP)Cl-PhIO-1-MeIm system. This indicates that the Mn(TPP)Cl-O<sub>2</sub>-Zn-AcOH-1-MeIm system involves a (1-MeIm)Mn(V):O active oxygen species. This system was successfully used for the conversion of .alpha.-ionone to the corresponding epoxides and allylic ketone and of di-Bu thioether to its sulfoxide with high yields and without any denaturation of the catalyst.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for epoxidn. of cyclooctene)

L58 ANSWER 24 OF 47 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1995:351792 HCPLUS  
 DOCUMENT NUMBER: 122:159793  
 TITLE: Selective oxidations in organic chemistry using biomimetic catalysts  
 AUTHOR(S): Mansuy, Daniel  
 CORPORATE SOURCE: Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques, Universite Rene Descartes, Paris, 75270/06, Fr.  
 SOURCE: New Aspects Org. Chem. II, Proc. Int. Kyoto Conf., 5th (1992), Meeting Date 1991, 477-97. Editor(s): Yoshida, Zen-ichi; Ohshiro, Yoshiki. Kodansha: Tokyo, Japan.  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB New selective oxidn. catalysts mimicking cytochrome P 450-dependent monooxygenases have been obtained by following three strategies. The first one was based on Fe(III) or Mn(III) porphyrins as homogeneous catalysts in the presence of an oxygen atom donor like PhIO or H2O2. Good results have been obtained for the hydroxylation of linear alkanes and the oxidn. of methoxyarenes to quinones by using iron porphyrins bearing electron-withdrawing substituents on the pyrrole .beta.-positions. The second strategy was to prep. supported catalysts by incorporation of a metalloporphyrin in a polymer mineral matrix (covalent binding or adsorption on silica, intercalation into layered clays...). The biotechnol. catalysts prepd. after the third strategy have been obtained by expression of the genes coding for different human liver cytochrome P 450 isoenzymes in yeast. The specific properties of these various catalysts are compared.

L58 ANSWER 25 OF 47 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1992:83060 HCPLUS  
 DOCUMENT NUMBER: 116:83060  
 TITLE: Biomimetic activation of the carbon-hydrogen bond. 2. Oxygenation of hydrocarbons with O2 catalyzed by porphyrin metal complexes in the presence of ferrocene as reducing agent  
 AUTHOR(S): Shul'pin, G. B.; Druzhinina, A. N.  
 CORPORATE SOURCE: Inst. Khim. Fiz. im. Semenova, Moscow, USSR  
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1991), (12), 2739-44  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Oxidn. of cyclohexane in the presence of metalloporphyrins, ferrocene, and O2 afforded cyclohexanol and cyclohexanone in varying degrees after an induction time; use of non-metal-contg. tetraphenylporphyrin resulted in a prolonged induction time followed by rapid oxidn.; use of benzylferrocene resulted in selectivity for cyclohexanol in higher overall product yield, as well as diminished induction period. PhEt afforded 1-phenylethanol and acetophenone; styrene afforded PhCHO, and metal effects on the rate of metalloporphyrin-catalyzed prodn. of PhCHO were studied. The parameter .phi. representing relative reactivity of C-H bonds in PhEt vs. cyclohexane was a sensitive function of reducing agent for a given catalyst and nearly coincided with .phi. that characterized hydroxylation reactions with hydroxyl radical.

IT 14172-90-8 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, for hydrocarbon oxidn. with oxygen in presence of ferrocene-derived reducing agents, biomimetic)

L58 ANSWER 26 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1991:655433 HCPLUS  
 DOCUMENT NUMBER: 115:255433  
 TITLE: Catalysis by metal porphyrins of the oxidation of unsaturated hydrocarbons in the presence of inverse micelles  
 AUTHOR(S): Borovkova, S. Yu.; Solov'eva, A. B.; Genkin, M. V.; Davydov, R. M.  
 CORPORATE SOURCE: Inst. Khim. Fiz. im. Semenova, Moscow, USSR  
 SOURCE: Zhurnal Fizicheskoi Khimii (1991), 65(8), 2279-83  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB Inverse micelles [of CTAB and Na bis(2-ethylhexyl)sulfosuccinate] in org. solvent mixts. increased the rate of oxidn. of unsatd. hydrocarbons (cholesterol, anthracene) catalyzed by the metalloporphyrin (e.g., tetraphenylporphyrinomagnesium chloride)-NaBH4-O2 system in a narrow range of concn.; product distributions varied little, if at all. The concn. range for surfactant acceleration of the oxidn. rate significantly exceeded the crit. micelle concn. (cmc) for each surfactant studied; moreover, at fixed surfactant concn. > cmc, the rate was extremal in metalloporphyrin concn. These observations were interpreted in terms of reagent partition between the org. and micellar phases, as well as isolation of the active system (consisting of metalloporphyrin, oxygen, and substrate) from cyclic hydroperoxides (which destroy the metalloporphyrin).

IT 14172-90-8 16456-81-8  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, in presence of inverse micelles, for oxidn. of unsatd. hydrocarbons)

L58 ANSWER 27 OF 47 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1991:188007 HCPLUS  
 DOCUMENT NUMBER: 114:188007  
 TITLE: Production of detergent range alcohols and ketones from alkanes using porphyrin catalysts  
 INVENTOR(S): Sanderson, John R.; Marquis, Edward T.; Payton, Howard F.  
 PATENT ASSIGNEE(S): Texaco Chemical Co., USA  
 SOURCE: U.S., 11 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4978799	A	19901218	US 1989-428812	19891030
EP 426290	A2	19910508	EP 1990-310155	19900917
EP 426290	A3	19910925		
R: DE, FR, GB, IT				
JP 03169831	A2	19910723	JP 1990-290985	19901030
PRIORITY APPLN. INFO.:				
			US 1989-428701	19891030
			US 1989-428703	19891030
			US 1989-428812	19891030

AB The reaction of C10-18 alkanes with a hydroperoxide, esp. tert-BuOOH or cumene hydroperoxide (I), in the presence of a transition metal (esp. Fe, Mn, or Co) porphyrin catalyst gives alcs. and ketones with minimal formation of byproducts. A mixt. of dodecane 50.0, chloroferroc phthalocyanine 0.10, and imidazole 0.07 g was treated slowly at 30.degree. with 80% I to give 5.02% dodecanones and 1.42% dodecanols.

IT 1643-19-2, Tetrabutylammonium bromide 14172-90-8  
 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for oxidn. of alkanes to alcs. and ketones)

L58 ANSWER 28 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1990:197650 HCPLUS  
DOCUMENT NUMBER: 112:197650  
TITLE: Metallocporphyrin-catalyzed oxidation of saturated hydrocarbons with sodium chlorite  
AUTHOR(S): Collman, James P.; Tanaka, Hiroo; Hembre, Robert T.; Brauman, John I.  
CORPORATE SOURCE: Dep. Chem., Stanford Univ., Stanford, CA, 94305-5080, USA  
SOURCE: Journal of the American Chemical Society (1990), 112(9), 3689-90  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 112:197650  
AB A remarkably efficient and active catalyst is formed when NaClO<sub>2</sub>, a manganese porphyrin, and an axial base such as 4-tert-butylypyridine are used in the oxidn. of satd. hydrocarbons. The unique reactivity of the chlorite-derived oxidant is contrasted with the active species formed by other shunt oxidants - in particular, hypochlorite. Mn(III)-porphyrin catalysis of chlorite disproportionation to chlorate and chloride is also reported.

L58 ANSWER 29 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1990:413600 HCPLUS  
DOCUMENT NUMBER: 113:13600  
TITLE: Functionalization of saturated hydrocarbons. Part XV. Electrochemical oxidation of saturated hydrocarbons by the Gif-Orsay system  
AUTHOR(S): Balavoine, G.; Barton, D. H. R.; Boivin, J.; Gref, A.; Hallery, I.; Ozbalik, N.; Pestana, J. A.; Riviere, H.  
CORPORATE SOURCE: Inst. Chim. Mol. Orsay, Univ. Paris-Sud, Orsay, 91405, Fr.  
SOURCE: New Journal of Chemistry (1990), 14, 175-83  
CODEN: NJCHE5; ISSN: 0398-9836  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The various components of the Gif-Orsay system for selective oxidn. of satd. hydrocarbons and their interactions with each other were examd. by cyclic voltammetry. This study permitted to establish the optimum conditions were detd. for preparative electroooxygenation of hydrocarbons and a mechanistic hypothesis was proposed where binuclear iron complexes were thought to intervene.  
IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(oxidn. catalysts, for electrochem. oxidn. of satd. hydrocarbons by Gif-Orsay system)

L58 ANSWER 30 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1989:631449 HCPLUS  
DOCUMENT NUMBER: 111:231449  
TITLE: Hydrocarbon oxidations catalyzed by azide- or nitride-activated metal coordination complexes  
INVENTOR(S): Ellis, Paul E.; Lyons, James E.; Myers, Harry K.  
PATENT ASSIGNEE(S): Sun Refining and Marketing Co., USA  
SOURCE: Eur. Pat. Appl., 21 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 11

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 274909	A2	19880720	EP 1987-311480	19871229
EP 274909	A3	19900207		
EP 274909	B1	19940810		
R: BE, DE, FR, GB, IT, NL				
US 4895682	A	19900123	US 1987-246	19870102
US 4895680	A	19900123	US 1987-247	19870102
CA 1302433	A1	19920602	CA 1987-553416	19871203
CA 1336188	A1	19950704	CA 1987-553420	19871203
NO 8705496	A	19880704	NO 1987-5496	19871230
NO 169710	B	19920421		
NO 169710	C	19920729		
SU 1833358	A3	19930807	SU 1987-4203962	19871231
JP 01180840	A2	19890718	JP 1988-46	19880104
JP 2517340	B2	19960724		
US 5663328	A	19970902	US 1996-672202	19960627
US 1987-246 19870102				
US 1987-247 19870102				
US 1987-66666 19870626				
US 1989-425089 19891023				
US 1990-568116 19900816				
US 1994-303106 19940907				

## PRIORITY APPLN. INFO.:

OTHER SOURCE(S): CASREACT 111:231449

AB The title process is used in the prepn. of alcs., ketones, acids, esters, or mixts. thereof. For example, oxidn. of 7 g isobutane in C6H6 at 80.degree. and 75 psig O2 for 6 h in the presence of 0.025 mmol Co(L)N3 [L = 1,3-bis(2-pyridylimino)isoindoline] gave a turn over no. of 196 which was quite superior to Co(L)(OAc) or Co(acac)2 with added NaN3. Products were Me3COH and Me2CO.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for oxidn. of hydrocarbons)

L58 ANSWER 31 OF 47 HCPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1988:630002 HCPLUS  
DOCUMENT NUMBER: 109:230002  
TITLE: Monooxygenase-like oxidation of hydrocarbons by hydrogen peroxide catalyzed by manganese porphyrins and imidazole: selection of the best catalytic system and nature of the active oxygen species

AUTHOR(S): Battioni, P.; Renaud, J. P.; Bartoli, J. F.; Reina-Artiles, M.; Fort, M.; Mansuy, Daniel

CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., CNRS, Paris, 75270, Fr.

SOURCE: Journal of the American Chemical Society (1988), 110(25), 8462-70

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:230002

AB Fe and Mn porphyrins alone are almost unable to catalyze cyclooctene epoxidn. or cyclooctane hydroxylation by H2O2. In the presence of imidazole, Mn(III) porphyrins, and particularly Mn(TDCPP)Cl, are much better catalysts than Fe porphyrins for oxygen-atom transfer from H2O2 to hydrocarbons. From a study of various Mn porphyrin catalysts and nitrogen base cocatalysts, the most efficient system that has been selected involves Mn(TDCPP)Cl in the presence of 10-20 equiv of imidazole. This system leads to high yields of alkene epoxidn. (90-100% in less than 1 h at room temp.). Epoxidn. of 1,2-dialkylethylenes is stereospecific and corresponds to a syn addn. of an oxygen atom to the double bond. This

system also leads to the oxidn. by H<sub>2</sub>O<sub>2</sub> of various alkanes such as cyclohexane, cyclooctane, adamantane, ethylbenzene or tetralin, with formation of the corresponding alcs. and ketones in yields between 40 and 80%. The Mn(TDCPP)Cl-imidazole-PhIO and Mn(TDCPP)Cl-imidazole-H<sub>2</sub>O<sub>2</sub> systems exhibit the following: (i) identical stereospecificities for the epoxidn. of stilbene and hex-2-ene, (ii) identical regioselectivities for the epoxidn. of isoprene and limonene as well as for the hydroxylation of n-heptane, and (iii) almost identical chemoselectivities for the oxidn. of cyclohexene and of mixts. of cyclooctane. This indicates that very similar, if not identical, high-valent Mn-oxo-intermediates are the active oxygenating species in both systems. Thus, thanks to the presence of imidazole, it is possible to perform efficient biomimetic monooxygenations of hydrocarbons by using the Mn(TDCPP)Cl catalyst and H<sub>2</sub>O<sub>2</sub> instead of PhIO as the oxygen-atom donor.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalytic activity of, in oxidn. of hydrocarbons)

L58 ANSWER 32 OF 47 HCAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1986:11084 HCAPLUS  
DOCUMENT NUMBER: 104:11084  
TITLE: Steric and electronic control of iron porphyrin  
catalyzed hydrocarbon oxidations  
AUTHOR(S): Nappa, Mario J.; Tolman, Chadwick A.  
CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and  
Co., Inc., Wilmington, DE, 19898, USA  
SOURCE: Inorganic Chemistry (1985), 24(26), 4711-19  
CODEN: INOCAJ; ISSN: 0020-1669  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The yields and product distributions in the oxidn. of hydrocarbons (cyclohexane, pentane, octane, methylcyclohexane, tert-butylcyclohexane, and ethylbenzene), with substituted Fe tetraphenylporphyrins and iodosobenzene, are affected by the nature and location of Ph ring substituents. These substrates were used to measure the activity, regioselectivity, substrate selectivity, and stereoselectivity of these substituted Fe porphyrin catalysts. Higher yields are obsd. with Fe porphyrins having bulky substituents near the Fe center. Kinetics measurements and concn. studies show that these substituents improve lifetimes by hindering catalyst bimol. self-destruction. Higher yields are also obsd. with electron-withdrawing substituents. A new Fe fluoro-pocket porphyrin shows high activity due to this electronic effect. Substrate and regioselectivity are also influenced by steric and electronic effects of the Fe porphyrin Ph ring substituents. Bulky porphyrins also affect the stereoselectivity at the 2-, 3- and 4-positions in tert-butylcyclohexane oxidn. A mechanism supported by kinetic modeling studies is proposed for the oxidn. reactions.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for oxidn. of hydrocarbons)

L58 ANSWER 33 OF 47 HCAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1983:504796 HCAPLUS  
DOCUMENT NUMBER: 99:104796  
TITLE: Conversion of an alkane to a mixture of an alcohol and a ketone  
INVENTOR(S): Middleton, Anthony Robert; Smith, David John Harry  
PATENT ASSIGNEE(S): British Petroleum Co. PLC, UK  
SOURCE: Eur. Pat. Appl., 14 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 79705	A1	19830525	EP 1982-305724	19821028
R: BE, DE, FR, GB, IT, NL				
US 4459427	A	19840710	US 1982-436785	19821026
AU 8289819	A1	19830505	AU 1982-89819	19821027
CA 1215388	A1	19861216	CA 1982-414477	19821029
JP 58085827	A2	19830523	JP 1982-192351	19821101
PRIORITY APPLN. INFO.:			GB 1981-32870	19811031
			GB 1981-32871	19811031

AB Alkanes were oxidized by hydrocarbyl hydroperoxides using a Fe or Mn square planar complex that had heterocyclic N donor ligands and weakly coordinating, non-coordinating, or no axial ligands, to give alcs. and ketones. Thus cyclohexane was treated with Me<sub>3</sub>COOH and Fe(tetraphenylporphyrin) to give 18% cyclohexanol and 35% cyclohexanone.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(oxidn. catalyst, for hydrocarbons with hydroperoxides)

L58 ANSWER 34 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1983:521435 HCPLUS

DOCUMENT NUMBER: 99:121435

TITLE: Catalytic replacement of unactivated alkane carbon-hydrogen bonds with carbon-X bonds (X = nitrogen, oxygen, chlorine, bromine, or iodine). Coupling of intermolecular hydrocarbon activation by MnIII TPPX complexes with phase-transfer catalysis

AUTHOR(S): Hill, Craig L.; Smegal, John A.; Henly, Timothy J.

CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA

SOURCE: Journal of Organic Chemistry (1983), 48(19), 3277-81  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:121435

AB The title reaction system is composed of 2 liq. phases and the oxidant PhIO. The alkane substrate, the MnIII TPPX catalyst, and the org. solvent (CH<sub>2</sub>C<sub>12</sub>, PhCl, or other arom. hydrocarbon) constitute 1 phase, a satd. aq. soln. of the Na salt of the anion to be incorporated into the alkane constitutes the 2nd phase, and the sparingly sol. PhIO constitutes a 3rd phase. When the 2 liq. phases and PhIO are stirred under an inert atm., both RX and ROH products are produced catalytically based on MnTPP, and in reasonable yield based on PhIO. The MnTPP moiety functions as a catalyst for C-H bond cleavage and for phase transfer of X- from the aq. phase to the org. phase, where the functionalization chem. takes place. ClO<sup>-</sup> can be used in place of, but is less effective than, PhIO, whereas H<sub>2</sub>O<sub>2</sub>, IO<sub>4</sub><sup>-</sup> and S<sub>2</sub>O<sub>8</sub><sup>2-</sup> are ineffective. Product distributions obtained from the oxidn. of cyclohexane, Me<sub>3</sub>CH, Me<sub>2</sub>CHCHMe<sub>2</sub> and PhCMe<sub>3</sub> are most consistent with a product-detg. step involving transfer of X from Mn to a free alkyl-radical intermediate.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for phase-transfer functionalization of alkanes in presence of iodosobenzene)

L58 ANSWER 35 OF 47 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1982:455050 HCPLUS

DOCUMENT NUMBER: 97:55050

TITLE: Biomimetic oxidation of organic sulfides with meso-tetraphenylporphyriniron chloride/imidazole/hydrogen peroxide

AUTHOR(S): Oae, Shigeru; Watanabe, Yoshihito; Fujimori, Ken

CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Ibaraki, 305, Japan  
 SOURCE: Tetrahedron Letters (1982), 23(11), 1189-92  
 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The enzyme model system meso-tetr phenylporphyriniron(III) chloride-imidazole catalyzed the S-oxygenation and oxidative S-dealkylation of org. sulfides with H2O2. The effect of para substitution on the rate of sulfoxidn. of PhSMe was studied. Electron-releasing groups accelerated S-oxidn., and there was good correlation between kinetics and 1-electron oxidn. potentials of the corresponding sulfides and with Brown-Okamoto .sigma.+ substituent consts.; the reaction const., .rho.+ was -0.26. Oxidn. of the benzothiophene I with this system gave the corresponding trans-sulfoxide stereoselectivity. Thus, this biomimetic oxidn. showed reasonable similarity to the enzymic oxidn. with cytochrome P-450.

IT 16456-81-8

RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, imidazole and, for oxidn. of org.  
 sulfides)

L58 ANSWER 36 OF 47 USPATFULL

ACCESSION NUMBER: 2003:47732 USPATFULL  
 TITLE: Main-group metal based asymmetric catalysts and applications thereof  
 INVENTOR(S): Jacobsen, Eric N., Boston, MA, United States  
 Sigman, Matthew S., Somerville, MA, United States  
 PATENT ASSIGNEE(S): President and Fellows of Harvard College, Cambridge, MA, United States (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 6521561 B1 20030218  
 APPLICATION INFO.: US 1998-71842 19980501 (9)  
 DOCUMENT TYPE: Utility  
 FILE SEGMENT: GRANTED  
 PRIMARY EXAMINER: Wood, Elizabeth D.  
 LEGAL REPRESENTATIVE: Gordon, Dana M., Foley Hoag LLP  
 NUMBER OF CLAIMS: 35  
 EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)  
 LINE COUNT: 2398  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to a method and catalysts for the stereoselective addition of a nucleophile to a reactive .pi.-bond of a substrate. The chiral, non-racemic catalysts of the present invention constitute the first examples of catalysts for nucleophilic additions that comprise a main-group metal and a tri- or tetra-dentate ligand.

L58 ANSWER 37 OF 47 USPATFULL

ACCESSION NUMBER: 2002:119566 USPATFULL  
 TITLE: Stabilized proteins  
 INVENTOR(S): Marshall, Christopher P., Brooklyn, NY, UNITED STATES  
 Hoffman, Alexander, Los Angeles, CA, UNITED STATES  
 Errico, Joseph P., Far Hills, CA, UNITED STATES  
 Marshall, Paul B., Munich, GERMANY, FEDERAL REPUBLIC OF

NUMBER	KIND	DATE
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PATENT INFORMATION: US 2002061549 A1 20020523  
 APPLICATION INFO.: US 2001-837235 A1 20010418 (9)  
 RELATED APPLN. INFO.: Continuation-in-part of Ser. No. WO 2000-US28595, filed on 16 Oct 2000, UNKNOWN

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-159763P	19991015 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	PENNIE AND EDMONDS, 1155 AVENUE OF THE AMERICAS, NEW YORK, NY, 100362711	
NUMBER OF CLAIMS:	20	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	26	Drawing Page(s)
LINE COUNT:	5385	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention described herein comprises methods for stabilizing polypeptides and polypeptide complexes, and the polypeptides and polypeptide complexes stabilized using the methods. To achieve stabilization, a cross-link reaction is controlled such that polypeptides and polypeptide complexes maintain their original functionality. In one embodiment, the invention provides a method for the identification of amino acid residues which, when cross-linked, are least disruptive to the structure and function of the polypeptide or polypeptide complex. In another embodiment, the invention provides a method for mutagenesis of identified residues to further control the cross-link reaction. Polypeptides and polypeptide complexes so stabilized can be utilized under a wide variety of physiological and non-physiological conditions. Further, the cross-link methodology disclosed herein may preclude the need for addition of exogenous structures to engineered proteins and complexes, such as peptide linkers that could be immunogenic and/or significantly decrease efficacy. In another embodiment, the invention provides a method for statistical analysis of databases of structural and/or sequence information available for polypeptides and polypeptide complexes to be stabilized. The statistical analysis identifies suitable residue pairs which are least likely to be disruptive of structure and function when cross-linked. Further, in a polypeptide chain or chains to be cross-linked, potentially undesirable reactive side-chains may be masked and protected, or altered using site-directed mutagenesis, e.g., to introduce a maximally conservative point mutation that will not support the cross-link reaction. The cross-link reaction conditions may also be adjusted to prevent undesired cross-links or other undesired side-effects. At residues identified as desirable positions for cross-linking, reactive side-chains may be introduced by site-directed mutagenesis, and the cross-link reaction is carried out using the conditions identified above.

L58 ANSWER 38 OF 47 USPATFULL  
 ACCESSION NUMBER: 2002:137161 ·USPATFULL  
 TITLE: Non-genotoxic metalloporphyrins as synthetic catalytic scavengers of reactive oxygen species  
 INVENTOR(S): Meunier, Bernard, Castanet, FRANCE  
 PATENT ASSIGNEE(S): Cosledan, Frederic, Escalquens, FRANCE  
 Eukarion, Inc., Bedford, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6403788	B1	20020611
APPLICATION INFO.:	US 2000-613891		20000711 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Raymond, Richard L.		
ASSISTANT EXAMINER:	Habte, Kahsay		
LEGAL REPRESENTATIVE:	Hamilton, Brook, Smith & Reynolds, P.C.		

NUMBER OF CLAIMS: 39  
 EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 2 Drawing Figure(s); 2 Drawing Page(s)  
 LINE COUNT: 1759

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to compounds which are non-genotoxic metalloporphyrins. These compounds are synthetic catalytic scavengers of reactive oxygen chemical species. The invention also relates to pharmaceutical compositions comprising these compounds and to methods of use of these compounds for preventing or arresting free radical associated diseases or conditions.

L58 ANSWER 39 OF 47 USPATFULL

ACCESSION NUMBER: 2002:88274 USPATFULL  
 TITLE: Biomimetic reagent system and its use  
 INVENTOR(S): Bather, Wolfgang, Lubeck, GERMANY, FEDERAL REPUBLIC OF  
 Duchstein, Hans-Jurgen, Pinneberg, GERMANY, FEDERAL  
 REPUBLIC OF  
 Hoffmann, Susanne, Buchholz, GERMANY, FEDERAL REPUBLIC  
 OF  
 PATENT ASSIGNEE(S): Drager Sicherheitstechnik GmbH, GERMANY, FEDERAL  
 REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6376254	B1	20020423
APPLICATION INFO.:	US 1999-394969		19990910 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 1999-19912380	19990319
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Snay, Jeffrey	
LEGAL REPRESENTATIVE:	McGlew and Tuttle, P.C.	
NUMBER OF CLAIMS:	30	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	1 Drawing Figure(s); 1 Drawing Page(s)	
LINE COUNT:	480	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A biomimetic reagent system is provided containing an oxygen donor and a catalyst based on porphyrin, which are applied to a carrier. A device that contains the system is also provided for determining components of gas or vapor samples, especially aromatics, such as benzene. A process for hydroxylating aromatics, such as benzene, using the biomimetic reagent system is also provided.

L58 ANSWER 40 OF 47 USPATFULL

ACCESSION NUMBER: 2001:86409. USPATFULL  
 TITLE: Methanol tolerant catalyst material  
 INVENTOR(S): Chu, Dervn, Havertown, PA, United States  
 Jiang, Rongzbong, Gaithersburg, MD, United States  
 PATENT ASSIGNEE(S): The United States of America as represented by the  
 Secretary of the Army, Washington, DC, United States  
 (U.S. government)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6245707	B1	20010612
APPLICATION INFO.:	US 1999-429702		19991028 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Wood, Elizabeth D.		

LEGAL REPRESENTATIVE: Clohan, Jr., Paul S.  
 NUMBER OF CLAIMS: 16  
 EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 9 Drawing Figure(s); 9 Drawing Page(s)  
 LINE COUNT: 639

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methanol tolerant catalyst materials and a method of making the same are provided. These novel catalyst materials are obtained by mixing together and heat-treating at least two different transition-metal-containing nitrogen chelates. In preferred embodiments, the nitrogen chelates comprise metalloporphyrins such as transition-metal-containing tetraphenylporphyrins. Preferred transition metals are iron, cobalt, nickel, copper, manganese, ruthenium, vanadium, and zinc, but could be any transition metal other than platinum or palladium. These materials offer improved catalytic oxygen reduction in the presence of methanol, as may occur at a fuel cell cathode after methanol crossover.

L58 ANSWER 41 OF 47 USPATFULL

ACCESSION NUMBER: 2000:128484 USPATFULL  
 TITLE: Octafluoro-meso-tetraarylporphyrins and methods for making these compounds  
 INVENTOR(S): DiMagno, Stephen G., Lincoln, NE, United States  
 PATENT ASSIGNEE(S): University of Nebraska-Lincoln, Lincoln, NE, United States (U.S. corporation)

NUMBER            KIND            DATE

PATENT INFORMATION:	US 6124452	20000926
APPLICATION INFO.:	US 1997-994891	19971219 (8)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Shah, Mukund J.	
ASSISTANT EXAMINER:	Sripada, Pavanaram K	
LEGAL REPRESENTATIVE:	Shook, Hardy & Bacon LLP	
NUMBER OF CLAIMS:	34	
EXEMPLARY CLAIM:	1	
LINE COUNT:	785	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The novel compounds of the present invention are .beta.-octafluoro-meso-tetraarylporphyrins of formula (I) and their metallic complexes of formula (II): ##STR1## .beta.-octafluoro-meso-tetraaryl porphyrins are synthesized by reacting 3,4-difluoropyrrole with an aromatic aldehyde in the presence of boron trifluoride etherate, followed by **oxidation**. The difluoropyrrole used in this reaction is produced by reacting 3,3,4,4-tetrafluoropyrrolidine or its corresponding salt, 3,3,4,4-tetrafluoropyrrolidinium salt, with a base such as potassium tert-butoxide. The metalloporphyrins of the present invention are synthesized by deprotonating .beta.-octafluoro-meso-tetraarylporphyrin ligands and treating said ligands with metal ions.

L58 ANSWER 42 OF 47 USPATFULL

ACCESSION NUMBER: 2000:106075 USPATFULL  
 TITLE: Catalyst that **oxidizes** steroids and other substrates with catalytic turnover  
 INVENTOR(S): Breslow, Ronald, Englewood, NJ, United States  
                   Yang, Jerry, New York, NY, United States  
                   Gabriele, Bartolo, New York, NY, United States  
 PATENT ASSIGNEE(S): The Trustees of Columbia University in the City of New York, New York, NY, United States (U.S. corporation)

NUMBER            KIND            DATE

PATENT INFORMATION:	US 6103892	20000815
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APPLICATION INFO.: US 1998-57417 19980408 (9)  
 DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted  
 PRIMARY EXAMINER: Kunz, Gary L.  
 LEGAL REPRESENTATIVE: White, John P. Cooper & Dunham LLP  
 NUMBER OF CLAIMS: 23  
 EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 11 Drawing Figure(s); 5 Drawing Page(s)  
 LINE COUNT: 678

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides a metallocporphyrin catalyst represented by the structure: ##STR1##

L58 ANSWER 43 OF 47 USPATFULL

ACCESSION NUMBER: 2000:21519 USPATFULL  
 TITLE: Metallocporphyrin **oxidation** catalyst covalently coupled to an inorganic surface and method making same  
 INVENTOR(S): Ying, Jackie Y., Winchester, MA, United States  
 Zhang, Lei, Cambridge, MA, United States  
 Sun, Tao, Midland, MI, United States  
 PATENT ASSIGNEE(S): Massachusetts Institute of Technology, Cambridge, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6028025		20000222
APPLICATION INFO.:	US 1996-734170		19961021 (8)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Straub, Gary P.		
ASSISTANT EXAMINER:	Vanoy, Timothy C		
LEGAL REPRESENTATIVE:	Wolf, Greenfield & Sacks, P.C.		
NUMBER OF CLAIMS:	25		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	23 Drawing Figure(s); 20 Drawing Page(s)		
LINE COUNT:	1111		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A system is provided including an article having a surface and a catalytic metal atom, capable of **oxidation**, covalently immobilized at the surface via a plurality of covalent bonds, but being free of direct covalent bonding to the surface. In particular, the invention relates to inorganic surfaces including silica, alumina, niobium **oxide**, or tantalum **oxide**, or a combination thereof and catalytic metal atoms including Fe, Mn, Cr, Ni, Co, Ru, and Os. The catalytic metal atom, covalently immobilized at the surface via a plurality of covalent bonds, can be immobilized via bonding through at least one atom that is bonded directly to the surface. The article preferably is an inorganic, mesoporous structure, in the pores of which are covalently bonded a plurality of metallocporphyrins. In particular, the catalytic metal atom, such as iron, manganese, chromium, nickel, cobalt, rhenium, and osmium are covalently bonded to a porphyrin structure which is bonded to an alumina or silica surface via bonds between the amine groups of the porphyrin structure of the alumina or silica surface. The invention also discloses supporting the catalytic metal atom bonded to the porphyrin structure via amine groups in the porphyrin and dopant atoms of the alumina or silica surface. Dopant atoms can include niobium and tantalum atoms.

L58 ANSWER 44 OF 47 USPATFULL

ACCESSION NUMBER: 1999:163881 USPATFULL  
 TITLE: Catalytic oxygenation of hydrocarbons by metallocporphyrin and metallosalen complexes

INVENTOR(S): Groves, John T., Princeton, NJ, United States

Carofiglio, Tommaso, Padua, Italy

Bonchio, Marcella, Padua, Italy

Sauve, Anthony, Princeton, NJ, United States

PATENT ASSIGNEE(S): The Trustees of Princeton University, Princeton, NJ, United States (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 6002026 19991214

APPLICATION INFO.: US 1996-760849 19961205 (8)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1996-686663, filed on 26 Jul 1996, now abandoned

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Kight, John

ASSISTANT EXAMINER: Desai, Rita

LEGAL REPRESENTATIVE: Hoffmann & Baron, LLP

NUMBER OF CLAIMS: 10

EXEMPLARY CLAIM: 1

NUMBER OF DRAWINGS: 5 Drawing Figure(s); 5 Drawing Page(s)

LINE COUNT: 964

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to novel **oxidative** processes for substrates such as olefins, alkanes, aromatics and alcohols using metallic porphyrin or salen catalytic complexes which have been specifically designed to maximize catalytic activity, thereby enhancing efficiency, selectively and speed of **oxidation** of these substrates. The choice of the substituents in the metallic complexes may be varied, but must be chosen to prevent specific ligand set arrangements known to be stable and therefore less catalytically efficient. Coordination complexes, particularly porphyrins and salens having nitrosyl axial ligands and electron-withdrawing peripheral substituents are preferred. Ruthenium coordination metals are the preferred metal center, with the highly reactive catalytic species found to be Ru.sup.III.

L58 ANSWER 45 OF 47 USPATFULL

ACCESSION NUMBER: 1998:88995 USPATFULL

TITLE: Process for the preparation of a mixture of guaiacol and p-methoxy phenol

INVENTOR(S): Moghe, Pramod Prabhakar, Pune, India

Ratnasamy, Paul, Pune, India

Raja, Robert, Madras, India

Pol, Ashwini Vinayak, Pune, India

Kotasthane, Madhav Gopal, Pune, India

Bahirat, Prakash Kondiba, Pune, India

PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, New Dehli, India (non-U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 5786519 19980728

APPLICATION INFO.: US 1996-602600 19960216 (8)

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Robinson, Allen J.

ASSISTANT EXAMINER: Badio, Barbara

LEGAL REPRESENTATIVE: Greenlee, Winner and Sullivan, P.C.

NUMBER OF CLAIMS: 14

EXEMPLARY CLAIM: 1

LINE COUNT: 434

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB An improved process is provided for the preparation of a mixture of guaiacol and p-methoxy phenol which comprises reacting anisole with hydrogen peroxide in the presence of a solid catalyst containing an organotransition metal complex wherein some or all of the hydrogen atoms of the said organotransition metal complex have been substituted by one or more electron withdrawing groups, and isolating the mixture of guaiacol and p-methoxy phenol formed.

L58 ANSWER 46 OF 47 USPATFULL

ACCESSION NUMBER: 97:18278 USPATFULL  
 TITLE: Porphyrins and metal complexes thereof having haloalkyl side chains  
 INVENTOR(S): Wijesekera, Tilak, Glen Mills, PA, United States  
 Lyons, James E., Wallingford, PA, United States  
 Ellis, Jr., Paul E., Downingtown, PA, United States  
 Bhinde, Manoj V., Boothwyn, PA, United States  
 PATENT ASSIGNEE(S): Sun Company, Inc. (R&M), Philadelphia, PA, United States (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 5608054 19970304  
 APPLICATION INFO.: US 1995-405684 19950317 (8)  
 RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1993-174732, filed on 29 Dec 1993 And a continuation-in-part of Ser. No. US 1993-175057, filed on 29 Dec 1993

DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted  
 PRIMARY EXAMINER: Datlow, Philip I.  
 LEGAL REPRESENTATIVE: Dickinson, Q. Todd, Falk, Stephen T.  
 NUMBER OF CLAIMS: 8  
 EXEMPLARY CLAIM: 1,8  
 NUMBER OF DRAWINGS: 7 Drawing Figure(s); 7 Drawing Page(s)  
 LINE COUNT: 384  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB Transition metal complexes of meso-haloalkylporphyrins, wherein the haloalkyl groups contain 2 to 8 carbon atoms have been found to be highly effective catalysts for **oxidation** of alkanes and for the decomposition of hydroperoxides.

L58 ANSWER 47 OF 47 USPATFULL

ACCESSION NUMBER: 96:101672 USPATFULL  
 TITLE: Porphyrins  
 INVENTOR(S): Wijesekera, Tilak, Glen Mills, PA, United States  
 Lyons, James E., Wallingford, PA, United States  
 Ellis, Jr., Paul E., Downingtown, PA, United States  
 PATENT ASSIGNEE(S): Sun Company, Inc. (R&M), Philadelphia, PA, United States (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION: US 5571908 19961105  
 APPLICATION INFO.: US 1993-174732 19931229 (8)  
 RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1990-568116, filed on 16 Aug 1990 which is a continuation-in-part of Ser. No. US 1989-425089, filed on 23 Oct 1989, now abandoned which is a continuation-in-part of Ser. No. US 1987-66666, filed on 26 Jun 1987, now patented, Pat. No. US 4900871 which is a continuation-in-part of Ser. No. US 1987-246, filed on 2 Jan 1987, now patented, Pat. No. US 4895682

DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted

PRIMARY EXAMINER: Datlow, Philip I.  
LEGAL REPRESENTATIVE: Dickinson, Q. Todd, Falk, Stephen T.  
NUMBER OF CLAIMS: 13  
EXEMPLARY CLAIM: 1  
LINE COUNT: 598

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention comprises new compositions of matter, which are iron, manganese, cobalt or ruthenium complexes of porphyrins having hydrogen, haloalkyl or haloaryl groups in meso positions, two of the opposed meso atoms or groups being hydrogen or haloaryl, and two of the opposed meso atoms or groups being hydrogen or haloalkyl, but not all four of the meso atoms or groups being hydrogen. The invention also comprises new compositions of matter in which all four of the meso positions are substituted with haloalkyl groups and the beta positions are substituted with halogen atoms. A new method of synthesizing porphyrinogens is also provided.

The novel compositions and others made according to the process of the invention are useful as hydrocarbon conversion catalysts; for example, for the **oxidation** of alkanes and the decomposition of hydroperoxides.

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FILE 'CASREACT' ENTERED AT 11:49:48 ON 15 MAY 2003  
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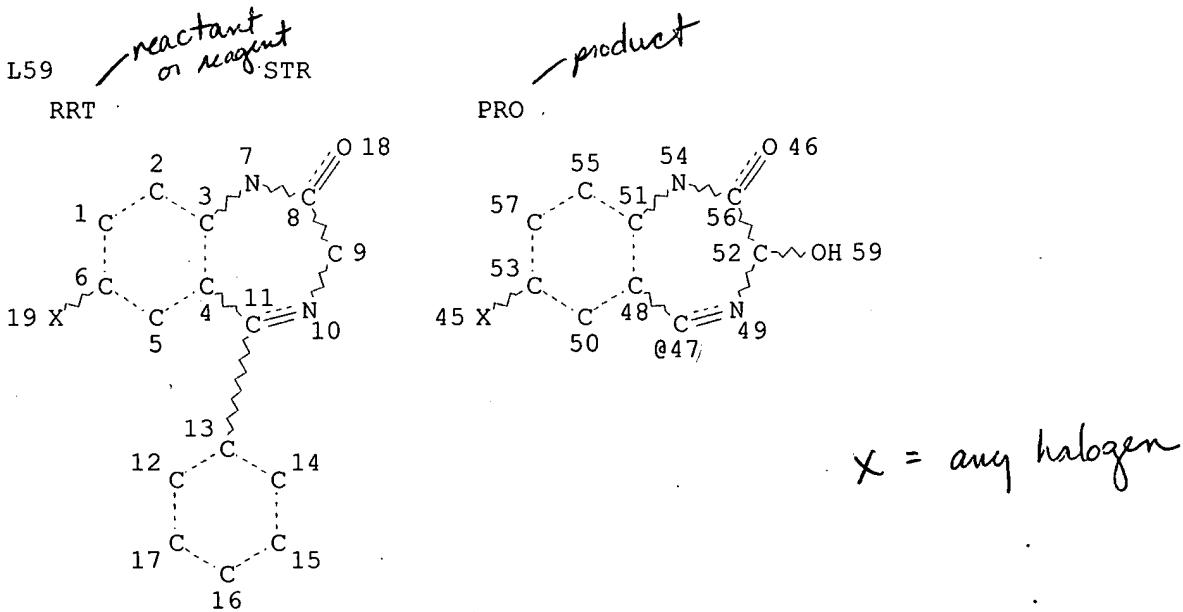
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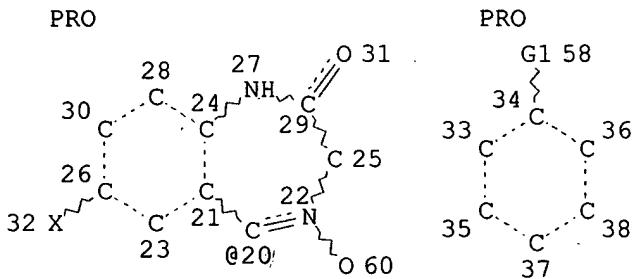
This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.



Page 1-A



Page 2-A

VAR G1=20/47

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 54

STEREO ATTRIBUTES: NONE  
L61 24 SEA FILE=CASREACT SSS FUL L59 ( 84 REACTIONS)

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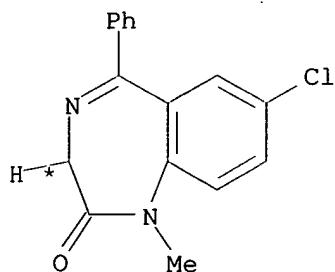
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L61 ANSWER 1 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 134:178573 CASREACT  
TITLE: Process for the metalloporphyrin catalyzed oxidation  
of organic compounds  
INVENTOR(S): Bernardelli, Patrick  
PATENT ASSIGNEE(S): Warner Lambert Company, USA  
SOURCE: PCT Int. Appl., 20 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

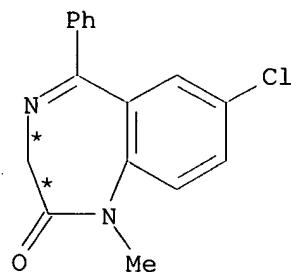
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809
PRIORITY APPLN. INFO.:			US 1999-148079P	19990810
			US 1999-150101P	19990820
			WO 2000-EP7726	20000809

AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, aprotic, polyhalogenated solvent (benzotrifluoride). Oxidn. of diazepam is conducted to mimic oxidn. (metab.) in biol. systems. The products of the oxidn. of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert aprotic solvent shows improved oxidn. yields when compared to prior art (e.g., CH<sub>3</sub>CN-CH<sub>2</sub>Cl<sub>2</sub>-water mixts.).

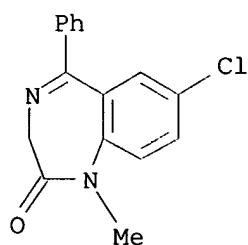
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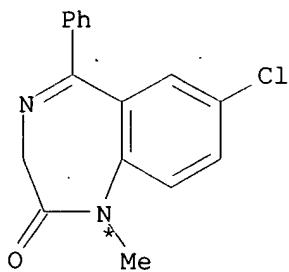
A



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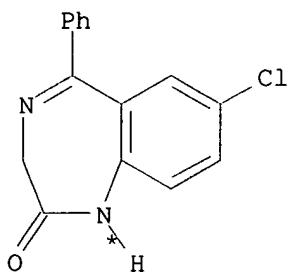


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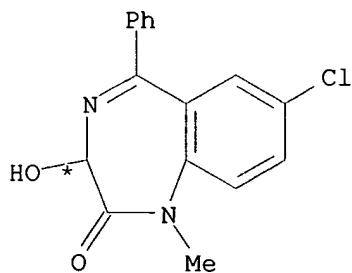


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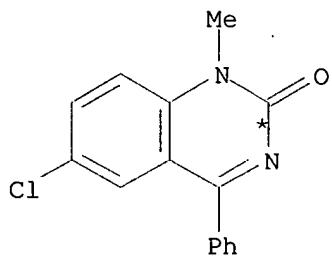
(1)



B  
YIELD 4%

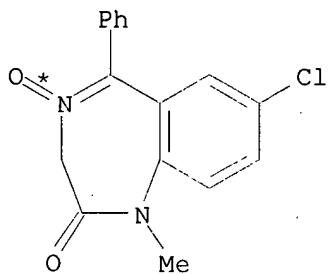


C  
YIELD 7%



D  
YIELD 1%





E  
YIELD 5%

RX(1) RCT A 439-14-5

STAGE(1)

SOL 98-08-8 Benzene, (trifluoromethyl)-

STAGE(2)

CAT 79968-43-7 Manganese, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-, 920-66-1 (F3C)2CHOH  
SOL 98-08-8 Benzene, (trifluoromethyl)-

STAGE(3)

RGT F 7722-84-1 H2O2  
SOL 7732-18-5 Water

STAGE(4)

CAT 288-32-4 1H-Imidazole  
SOL 7732-18-5 Water

STAGE(5)

CAT 631-61-8 NH4OAc  
SOL 7732-18-5 Water

PRO B 1088-11-5, C 846-50-4, D 20927-53-1, E 2888-64-4

NTE 1 EQUIV. PEROXIDE, PHASE-TRANSFER CATALYSIS

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 2 OF 24 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 129:290114 CASREACT

TITLE: Oxidation of nitrogen-containing heterocycles using biocatalysts

AUTHOR(S): Didenko, T. I.

CORPORATE SOURCE: A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, 270080, Ukraine

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1998), 47(8), 1565-1570

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Consultants Bureau

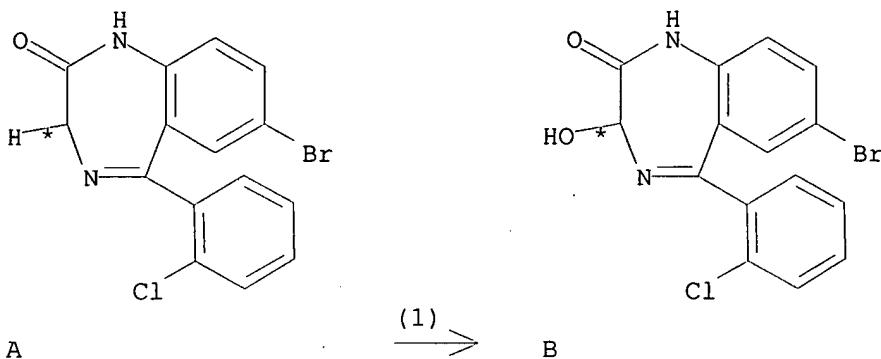
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for stereospecific hydroxylation of 1,2-dihydro-3H-1,4-benzodiazepin-2-ones using free and immobilized cells of Actinomycetes as

biocatalysts was developed. The hydroxylation under the action of yeast results in the formation of racemates. *Actinomyces* do not hydroxylate quinazolinones, quinoxalinones, and tetrahydro-1,5-benzodiazepin-2-ones; derivs. of 1,2,3,4-tetrahydro-1,5-benzodiazocin-2-ones are transformed into 2-[N-(3-acetylaminopropionyl)amino]benzophenones.

RX(1) OF 15      A    ==>    B



RX(1)      RCT A 51753-57-2  
 PRO B 214194-35-1  
 SOL 67-68-5 DMSO  
 NTE BIOTRANSFORMATION, ENZYMIC HYDROXYLATION, ACTINOMYCES  
 ROSEOCHROMOGENES

REFERENCE COUNT:      16      THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 3 OF 24    CASREACT    COPYRIGHT 2003 ACS

ACCESSION NUMBER:      122:10073    CASREACT

TITLE:      Method for production of 1,4-benzodiazepine  
 derivatives

INVENTOR(S):      Krawczynska, Bogumila; Morawski, Bogdan; Kalis,  
 Jadwiga; Chojnacka, Romualda

PATENT ASSIGNEE(S):      Tarchominskie Zaklady Farmaceutyczne "Polfa", Pol.

SOURCE:      Pol., 4 pp.

DOCUMENT TYPE:      Patent

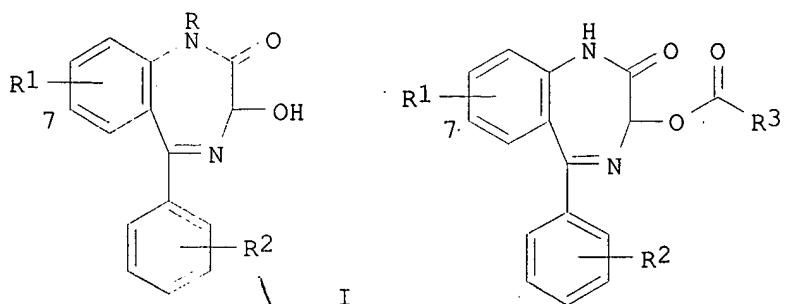
LANGUAGE:      Polish

FAMILY ACC. NUM. COUNT:      1

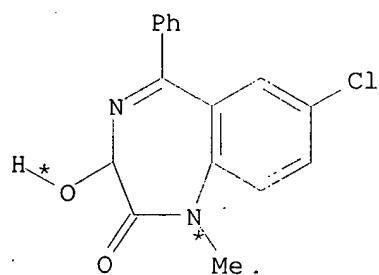
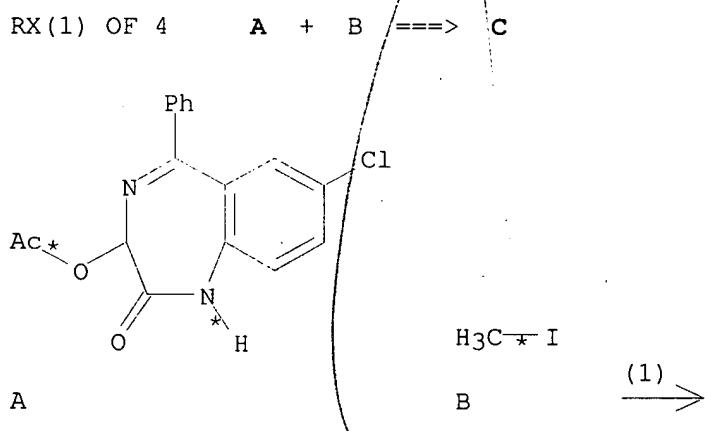
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 158635	B1	19920930	PL 1988-272101	19880427
PRIORITY APPLN. INFO.:			PL 1988-272101	19880427
OTHER SOURCE(S):		MARPAT 122:10073		

uses  
*includes solvent*  
*excluded by prov130*



AB Benzodiazepine derivs. I [R = (un)substituted C1-4 alkyl; R1, R2 = H, halo, nitro] are prep'd. by simultaneous hetero-phase hydrolysis and alkylation of benzodiazepine esters II [R3 = C1-3 alkyl] in a system comprising a water-insol. org. solvent and an aq. soln. of an alkali metal hydroxide, in the presence of a quaternary ammonium salt (phase-transfer catalyst), and under the action of an alkylating agent RX (X = halo). For example, a suspension of II [R1 = 7-Cl, R2 = H, R3 = Me] in a mixt. of CH<sub>2</sub>Cl<sub>2</sub>, aq. 40% NaOH, and Bu<sub>4</sub>N<sup>+</sup> Cl<sup>-</sup>, was stirred 1 h at 20-25.degree., dild. with H<sub>2</sub>O, treated dropwise with MeI, and stirred 3 h at 25-30.degree., to give I [R = Me, R1 = 7-Cl, R2 = H] in 85% yield with m.p. 159-160.degree.. A similar prep'n. using KOH and PhCH<sub>2</sub>N<sup>+</sup>Et<sub>3</sub> Cl<sup>-</sup> in ClCH<sub>2</sub>CH<sub>2</sub>Cl gave 89% yield. Also prep'd. were I [R = Me, R1 = 7-Cl, R2 = o-Cl] in 87% yield, and I.HCl [R = CH<sub>2</sub>CH<sub>2</sub>NET<sub>2</sub>, R1 = 7-Cl, R2 = o-F] in 79% yield.



C  
YIELD 85%

RX(1) RCT A 1824-74-4

## STAGE(1)

RGT D 1310-73-2 NaOH  
 CAT 1643-19-2 Bu4N.Br  
 SOL 7732-18-5 Water, 75-09-2 CH2C12

*Solvent excluded by proviso*

## STAGE(2)

RCT B 74-88-4  
 PRO C 846-50-4

L61 ANSWER 4 OF 24 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 114:246735 CASREACT

TITLE: Characteristics of charge transfer of  
1,4-benzodiazepin-2-ones

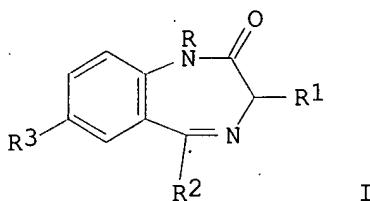
AUTHOR(S): Ying, Baining; Ouyang, Jiexiang; Xu, Xiangong

CORPORATE SOURCE: Dep. Chem., Zhongshan Univ., Guangzhou, 510275, Peop.  
Rep. ChinaSOURCE: Gaodeng Xuexiao Huaxue Xuebao (1990), 11(11), 1254-8  
CODEN: KTHPDM; ISSN: 0251-0790

DOCUMENT TYPE: Journal

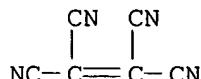
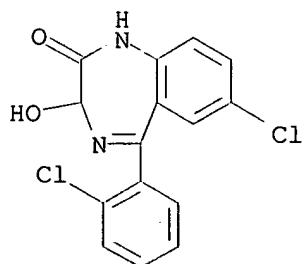
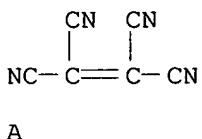
LANGUAGE: Chinese

GI



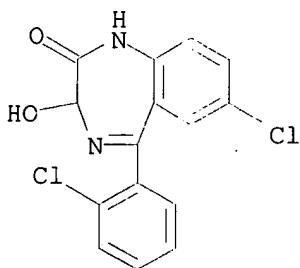
AB The interaction of 1,4-benzodiazepin-2-ones I (R = H, Me; R1 = H, OH, BzO, AcO; R2 = Ph, 2-pyridyl, 2-ClC6H4; R3 = H, Br, Cl, iodo, cyano, NO2, NH2, NHAc) with tetracyanoethylene or potassium p-methylphenoxyde can form charge transfer complexes. By a spectrophotometric method the electron affinity and the ionization potential of the title compds. are calcd. with the energy of electron transfer. The thermodn. consts. of the complexes are detd. as well. 1,4-Benzodiazepin-2-ones can act not only as charge acceptor but also as charge donor.

RX(17) OF 20 A + R ==&gt; S



(17)

S: CM 1

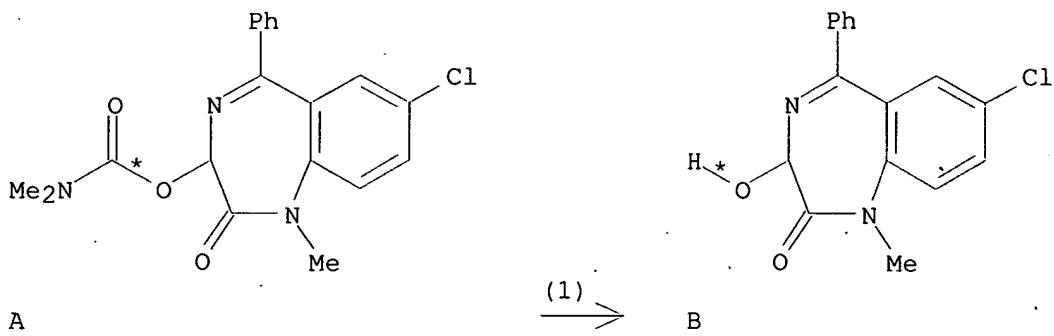


S: CM 2

RX(17) RCT A 670-54-2, R **846-49-1**  
PRO S **134070-75-0**

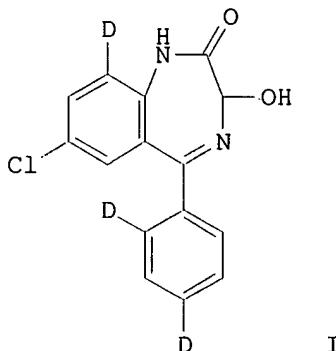
L61 ANSWER 5 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 114:220623 CASREACT  
TITLE: Voltammetric studies on the interactions between camazepam metabolic series and human serum albumin. Determination of oxazepam using adsorptive stripping voltammetry  
AUTHOR(S): Zapardiel, A.; Perez Lopez, J. A.; Bermejo, E.; Hernandez, L.; Chicharro, M.  
CORPORATE SOURCE: Dep. Anal. Chem., Auton. Univ., Madrid, 28049, Spain  
SOURCE: Analytica Chimica Acta (1991), 244(1), 49-57  
CODEN: ACACAM; ISSN: 0003-2670  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The behavior of oxazepam in adsorptive stripping voltammetry was studied taking into account those conditions which have an influence on the accumulation step (electrolyte, pH, time, potential, drop size and stirring rate), rest time and stripping step (pulse amplitude and scan rate). Oxazepam can be detd. at a hanging mercury drop electrode by differential-pulse voltammetry in 0.008 M Britton-Robinson buffer at pH 2.0 with a -0.50 V accumulation potential. Its detection limit was found to be 3.6 times. 10-10 M (30-s accumulation) and the relative std. deviation for oxazepam concns. in the range 2.8 times. 10-8-4.0 times. 10-7 M is lower than 2.8% (80-s accumulation). In addn., a procedure using adsorptive stripping voltammetry was developed to study the interactions occurring between human albumin and the camazepam metabolic series (camazepam, temazepam and oxazepam). The interactions decreased in the order temazepam > oxazepam > camazepam and the groups and structural modifications favoring interaction were detd.

RX(1) OF 1      A    ==&gt;   B



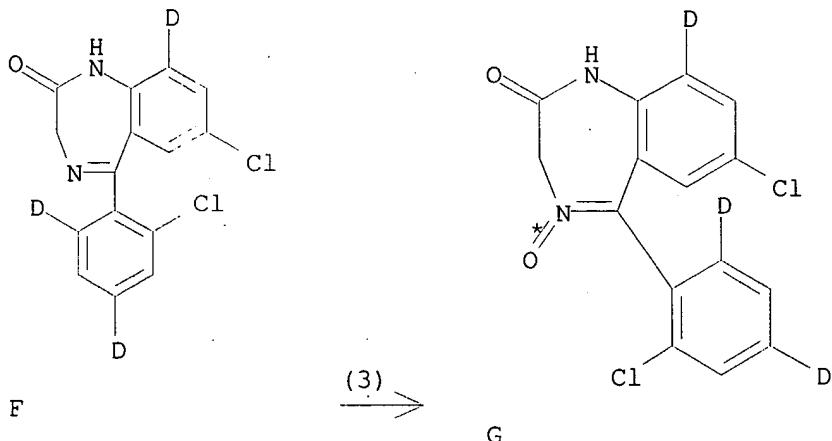
RX(1) RCT A 36104-80-0  
PRO B 846-50-4

L61 ANSWER 6 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 114:185445 CASREACT  
TITLE: Synthesis of deuterium labeled lorazepam  
AUTHOR(S): Koves, G. J.  
CORPORATE SOURCE: Cent. Forensic Sci., Toronto, ON, M7A 2G8, Can.  
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals  
(1991), 29(1), 15-22  
CODEN: JLCRD4; ISSN: 0362-4803  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



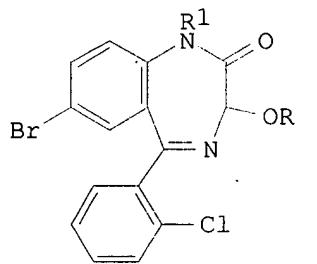
AB Synthesis of 2H3-lorazepam I was achieved by modification of literature procedures for the unlabeled drug. The key step in the seven step procedure was the selective exchange of 2-amino-5,2'-dichlorobenzophenone with deuterium in deuterated acids. Purifns. were carried out by preparative HPLC. I is suitable for use as an internal std. in GC-MS-NICI-SIM quant. anal. in forensic case work.

RX(3) OF 21 . . . F ==> G . . .



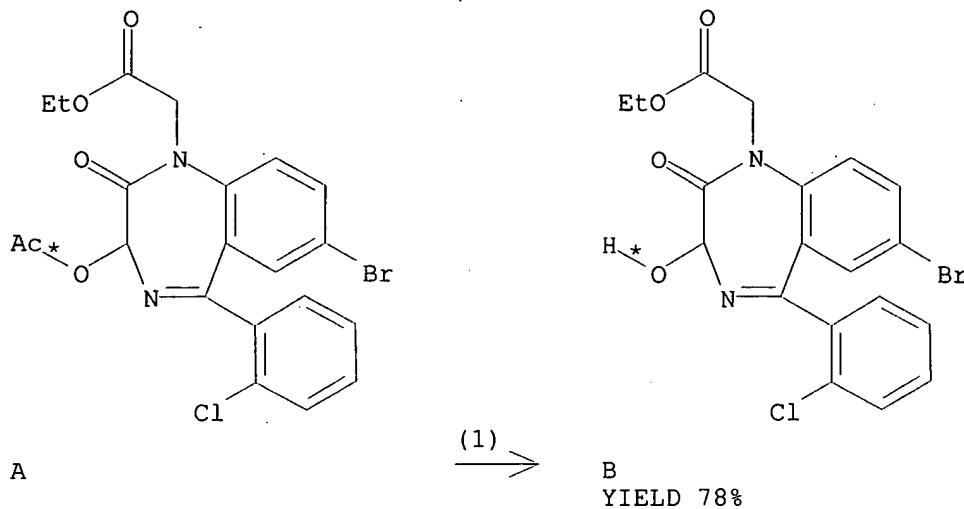
RX(3) RCT F 133358-31-3  
 PRO G 133358-32-4  
 CAT 937-14-4 MCPBA

L61 ANSWER 7 OF 24 CASREACT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 114:6467 CASREACT  
 TITLE: Basic hydrolysis of 3-acetoxy-7-bromo-5-(o-chlorophenyl)-1-(ethoxycarbonylmethyl)-1,2-dihydro-3H-1,4-benzodiazepin-2-one  
 AUTHOR(S): Mazurov, A. A.; Dvorkin, A. A.; Simonov, Yu. A.; Andronati, S. A.  
 CORPORATE SOURCE: Fiz.-Khim. Inst. im. Bogatskogo, Odessa, 270080, USSR  
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1990), (5), 685-90  
 CODEN: KGSSAQ; ISSN: 0453-8234  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB The ease of selective hydrolysis of title compd. I (R = Ac, R1 = CH2CO2Et) with 1 equiv of base to hydroxy ketone I (R = H, R1 same) was attributed to anchimeric assistance from the ethoxycarbonyl group. Hydrolysis with 2 equiv of base in aq. MeOH afforded the transesterification product I [R = H, R1 = CH2CO2Me (II)]. II crystd. from benzene in the P212121 space group; this guarantees that crystn. is accompanied by autoresoln., forming crystals of a single enantiomer. The crystal and mol. structure of II was detd. by x-ray crystallog.

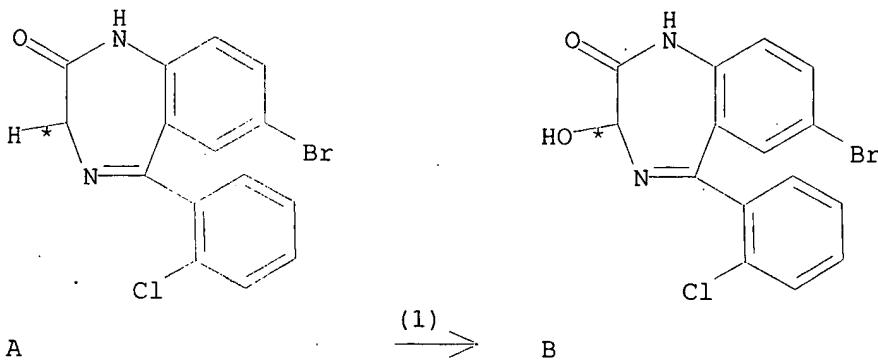
RX(1) OF 2      A    ==&gt;    B



RX(1)      RCT A 130788-45-3  
 RGT C 1310-73-2 NaOH  
 PRO B 130788-47-5  
 SOL 67-56-1 MeOH, 7732-18-5 Water  
 NTE Reaction products depend on conditions

L61 ANSWER 8 OF 24    CASREACT    COPYRIGHT 2003 ACS  
 ACCESSION NUMBER:      113:113735    CASREACT  
 TITLE:                    Microbial synthesis of 3-hydroxy derivatives of  
 1,4-benzodiazepine-2-ones  
 AUTHOR(S):              Davidenko, T. I.; Zabolotskaya, N. N.  
 CORPORATE SOURCE:       Fiz.-Khim. Inst., Odessa, USSR  
 SOURCE:                 Khimiko-Farmatsevticheskii Zhurnal (1990), 24(5), 65-7  
 CODEN: KHFZAN; ISSN: 0023-1134  
 DOCUMENT TYPE:          Journal  
 LANGUAGE:                Russian  
 AB    Strains of actinomyces and yeast which effectively accomplish  
 hydroxylation of 1,4-benzodiazepin-2-ones to form optically active compds.  
 were identified. The conditions for their hydroxylation were developed.  
 The hydroxylase system of *Saccharomyces cerevisiae* was shown to contain  
 cytochrome P 450 and NADPH-cytochrome-C-reductase. It was concluded that  
 the hydroxygenase system of actinomyces had specificity. The prepn. and  
 physicochem. properties of 8 new benzodiazepinones are reported.

RX(1) OF 8      A    ==&gt;    B



RX(1) RCT A 51753-57-2  
PRO B 70030-11-4

L61 ANSWER 9 OF 24 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER:

111:56925 CASREACT

TITLE:

Asymmetric transformation. II. Racemization reaction

of 1,4-benzodiazepinoxazole derivative

Okada, Yutaka; Takebayashi, Toyonori

CORPORATE SOURCE: Process Dev. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(10), 3787-92

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

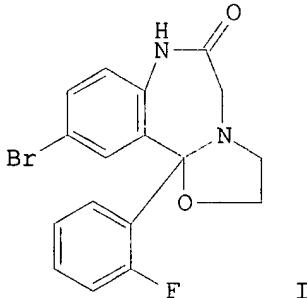
Journal

LANGUAGE:

English

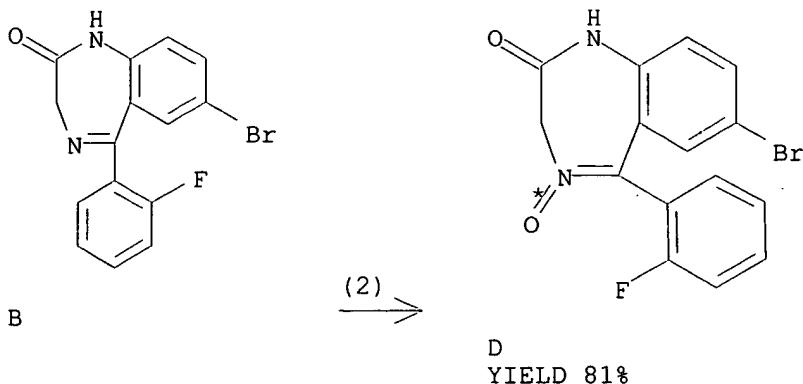
GI

*uses solvent  
excluded by proviso*



AB Optically active crystals of 10-bromo-11b-(2-fluorophenyl)-2,3,7,11b-tetrahydrooxazolo[3,2-d][1,4]benzodiazepin-6(5H)-one (I) were obtained by preferential crystn.; they were sometimes levorotatory and sometimes dextrorotatory. This phenomenon was an example of second-order asym. transformation between enantiomers. The rapid racemization reaction, essential for asym. transformation, was obsd. in MeOH. The decrease of optical rotation obeyed pseudo first-order kinetics, and the half-lives of the racemization in MeOH were 21 s at 30.degree., 37 s at 20.degree., and 70 s at 10.degree.. The mechanism and factors which affect the rate of the racemization are discussed.

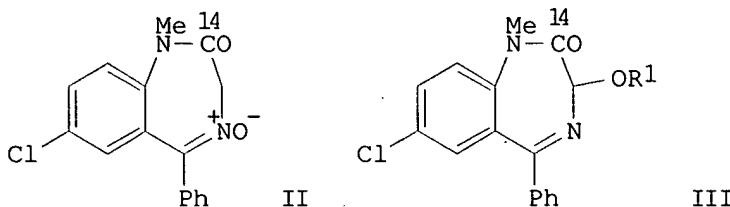
RX(2) OF 7 ...B ==> D...



RX (2)	RCT	B	2647-50-9
	RGT	E	79-21-0 ACOOH
	PRO	D	10329-38-1
	SOL		75-09-2 CH <sub>2</sub> Cl <sub>2</sub>

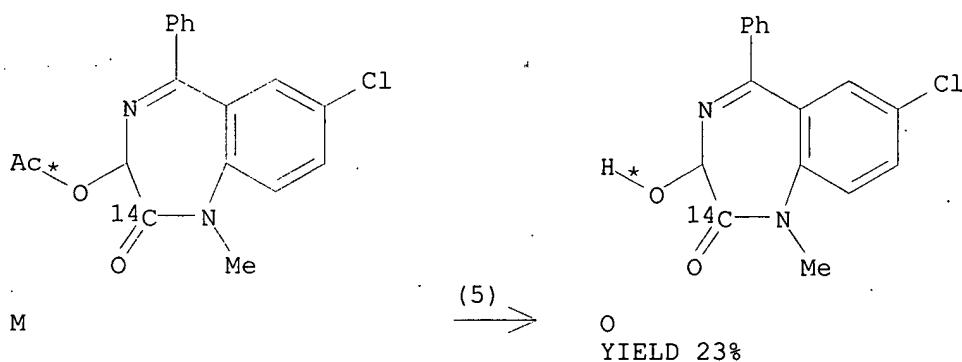
solvent except excluded by proviso

L61 ANSWER 10 OF 24    CASREACT    COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 107:217605    CASREACT  
TITLE: Synthesis of 7-chloro-1,3,-dihydro-3-hydroxy-1-methyl-  
5-phenyl-2H-1,4-benzodiazepin-2-one-2-14C  
(2-14C-temazepam)  
AUTHOR(S): Dain, Jeremy G.  
CORPORATE SOURCE: Dep. Drug Metab., Sandoz Res. Inst., East Hanover, NJ,  
07936, USA  
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals  
(1987), 24(5), 499-504  
CODEN: JLCRD4; ISSN: 0362-4803  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Condensation of  $\text{ClCH}_2\text{C}_1\text{4COCl}$  with  $5,2\text{-Cl}(\text{RNMe})\text{C}_6\text{H}_3\text{Bz}$  (I, R = H) gave amide I (R =  $14\text{COCH}_2\text{Cl}$ ). Cyclocondensation of  $\text{H}_2\text{NOH}$  and I (R =  $14\text{COCH}_2\text{Cl}$ ) gave benzodiazepine oxide II. II was converted to acetate III (R1 = Ac) with  $\text{Ac}_2\text{O}$  and hydrolyzed to the title compd. III (R1 = H) in 3.8% overall radiochem. yield.

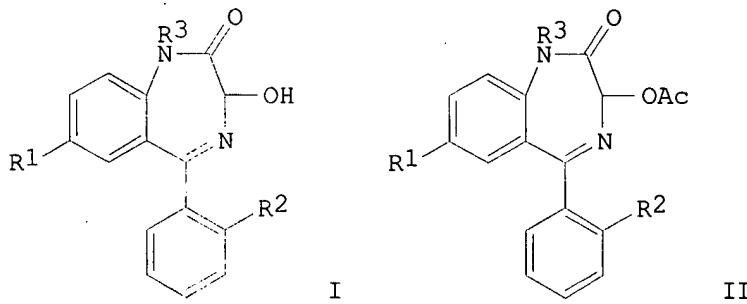
RX(5) OF 15 . . . M ==> O



RX(5) RCT M 111257-65-9  
 RGT P 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
 PRO O 111257-66-0  
 SOL 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

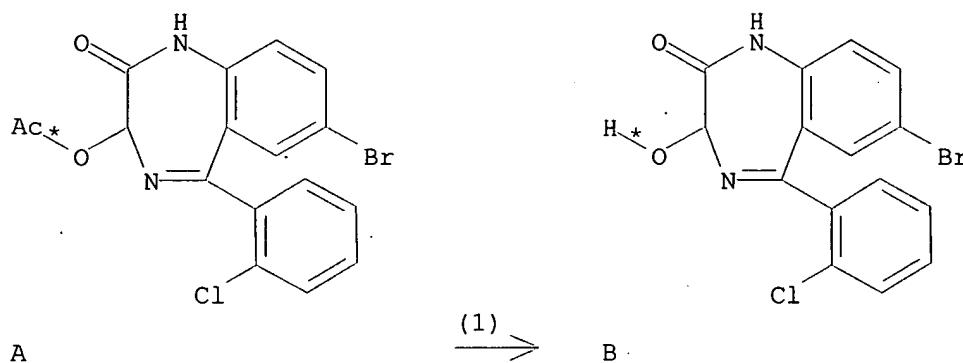
L61 ANSWER 11 OF 24 CASREACT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 105:191141 CASREACT  
 TITLE: 3-Hydroxy-1,3-dihydro-2H-1,4-benzodiazepin-2-ones  
 INVENTOR(S): Andronati, S. A.; Mazurov, A. A.; Dimitrishchuk, G. V.  
 PATENT ASSIGNEE(S): Physical-Chemical Institute, Academy of Sciences,  
 Ukrainian S.S.R., USSR  
 SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1985, (23), 86.  
 CODEN: URXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Russian  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1162800	A1	19850623	SU 1982-3543660	19821213
PRIORITY APPLN. INFO.:			SU 1982-3543660	19821213
GI				



AB The title compds. (I; R<sub>1</sub> = H, halo, C<sub>1</sub>-4 alkyl; R<sub>2</sub> = H, halo; R<sub>3</sub> = H, C<sub>1</sub>-4 alkyl) are prep'd. by reacting acetoxymethylbenzodiazepinones II with a deacylating agent. The prepn. of I is accelerated and simplified by using hydrazine hydrate as the deacylating agent, and by conducting the reaction at 40-60.degree. and pH 8-9.

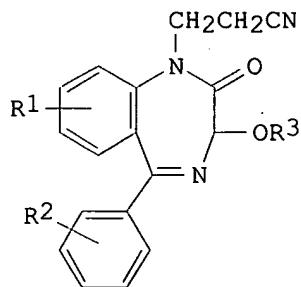
RX(1) OF 1                    A ==> B



RX(1) RCT A 70030-10-3  
PRO B 70030-11-4

L61 ANSWER 12 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 104:168499 CASREACT  
TITLE: Cyanoethylated 1,4-benzodiazepines  
INVENTOR(S): Schlager, Ludwig H.  
PATENT ASSIGNEE(S): Gerot-Pharmazeutika G.m.b.H., Austria  
SOURCE: Austrian, 5 pp.  
CODEN: AUXXAK  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

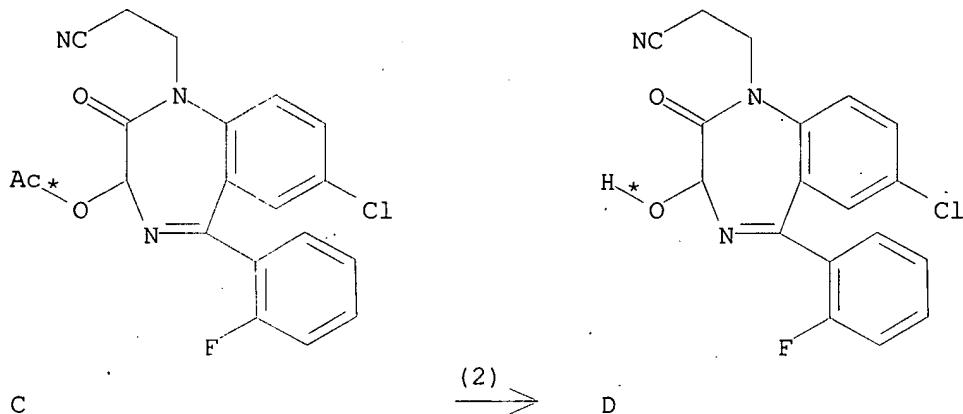
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 379391	B	19851227	AT 1984-150	19840118
AT 8400150	A	19850515		
ES 539059	A1	19851116	ES 1984-539059	19841226
NO 8500189	A	19850719	NO 1985-189	19850117
NO 161672	B	19890605		
NO 161672	C	19890913		
PRIORITY APPLN. INFO.:			AT 1984-150	19840118



AB Soporific (no data) title compds (I: R1 = H, CF<sub>3</sub>, halo, NO<sub>2</sub>; R2 = H, halo;

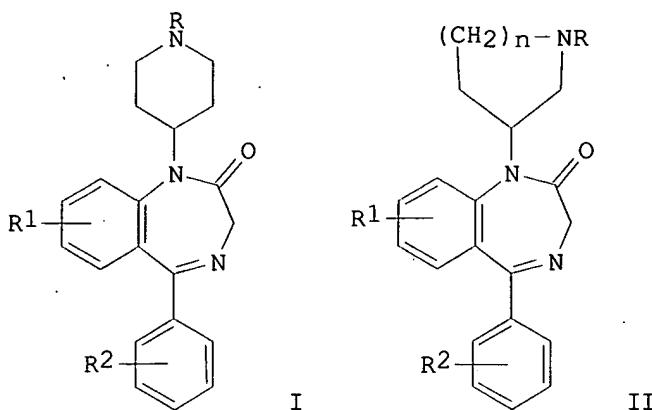
R3 = H) were prep'd. Thus, 3-(acetyloxy)-7-chloro-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one and CH<sub>2</sub>:CHCN were stirred at room temp. with a catalytic amt. of PhCH<sub>2</sub>N+Me<sub>3</sub>OH- to give 93.7% I (R1 = 7-Cl, R2 = 2-F, R3 = Ac) which was saponified to give 93% I (R1 = 7-Cl, R2 = 2-F, R3 = H).

RX(2) OF 3     ...C    ==>    D



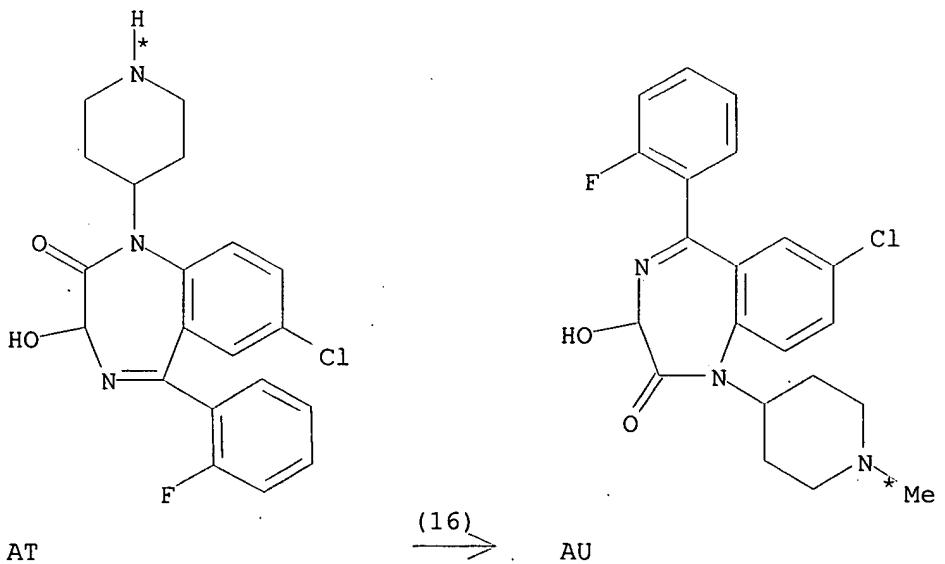
RX(2)     RCT    C 101661-96-5  
PRO    D 75696-02-5

L61 ANSWER 13 OF 24    CASREACT    COPYRIGHT 2003 ACS  
 ACCESSION NUMBER:    103:37458    CASREACT  
 TITLE:    1-Azacycloalkyl-1,4-benzodiazepin-2-ones with  
           antianxiety-antidepressant actions  
 AUTHOR(S):    Sugasawa, Tsutomu; Adachi, Makoto; Sasakura, Kazuyuki;  
           Matsushita, Akira; Eigyo, Masami; Shiomi, Teruo;  
           Shintaku, Haruyuki; Takahara, Yukio; Murata, Shunji  
 CORPORATE SOURCE:    Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka,  
           553, Japan  
 SOURCE:    Journal of Medicinal Chemistry (1985), 28(6), 699-707  
 DOCUMENT TYPE:    CODEN: JMCMAR; ISSN: 0022-2623  
 LANGUAGE:    English  
 GI



AB A series of 1-azacycloalkyl-1,4-benzodiazepin-2-ones I and II (R = H, Me, PhCH<sub>2</sub>CH<sub>2</sub>; R<sub>1</sub>, R<sub>2</sub> = H, halo; n = 1, 2) were synthesized from 1-azacycloalkyl-2-benzoylanilines and corresponding imines and then evaluated for their central nervous system activities. Pharmacol. data showed that some of these compds. have potent antidepressant properties, as assessed by their antagonism of tetrabenazine induced ptosis and their inhibition of [<sup>3</sup>H]norepinephrine uptake into rat brain synaptosomes, as well as their moderate antianxiety properties of preventing of pentylenetetrazol convulsion, suppressing conflict behavior, and displacing potential for [<sup>3</sup>H]diazepam binding. Secondary function of the azacyclic ring at position 1 was essential for the prodn. of the antidepressant properties. Of these new series, I (R = H; R<sub>1</sub> = R<sub>2</sub> = F) has the potential to become a useful antidepressant drug with a moderate antianxiety property.

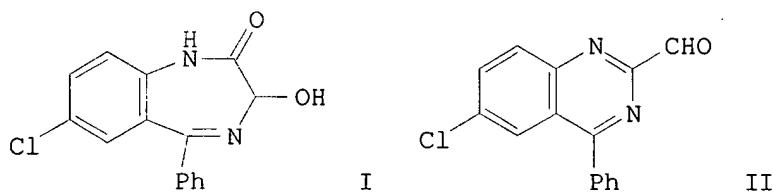
RX(16) OF 407 . . . AT ==> AU . . .



RX(16) RCT AT 96110-74-6  
RGT AV 77-78-1 Me<sub>2</sub>SO<sub>4</sub>, AW 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AU 96110-75-7

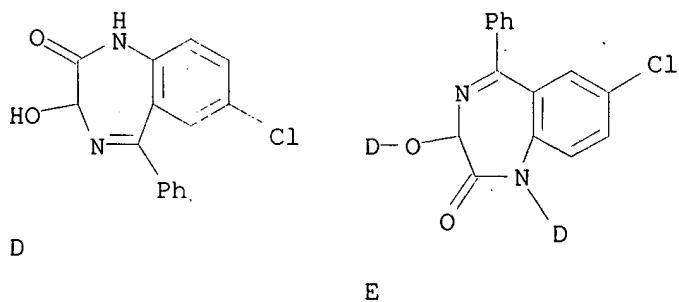
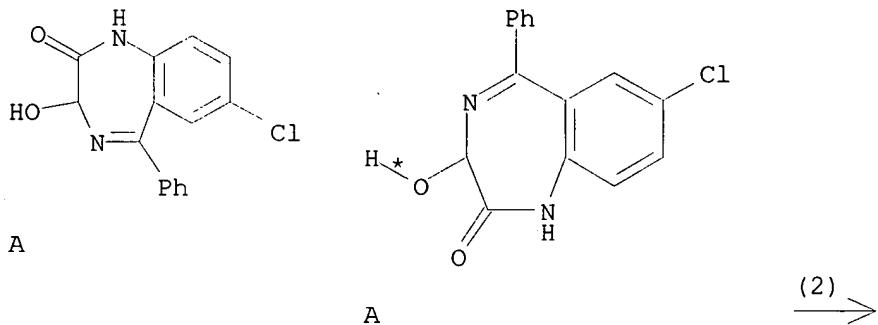
SOL 75-05-8 MeCN

L61 ANSWER 14 OF 24    CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER:    102:166099    CASREACT  
TITLE:                Quantitative [1,3,2,3]-elimination of water from  
                      oxazepam  
AUTHOR(S):           Kaupp, Gerd; Knichala, Bernd  
CORPORATE SOURCE:    Fachber. Chem.-Org. Chem., Univ. Oldenburg, Oldenburg,  
                      D-2900, Fed. Rep. Ger.  
SOURCE:              Chemische Berichte (1985), 118(2), 462-7  
DOCUMENT TYPE:       CODEN: CHBEAM; ISSN: 0009-2940  
LANGUAGE:            Journal  
GI



AB D-labeling expts. indicated that in the pyrolysis of oxazepam (I) at 150.degree. to give aldehyde II the H attached to C-3 in I becomes the formyl H in II. The mechanism is discussed. The O-Ac deriv. of I decomp. nonselectively at higher temps. with no II being detectable.

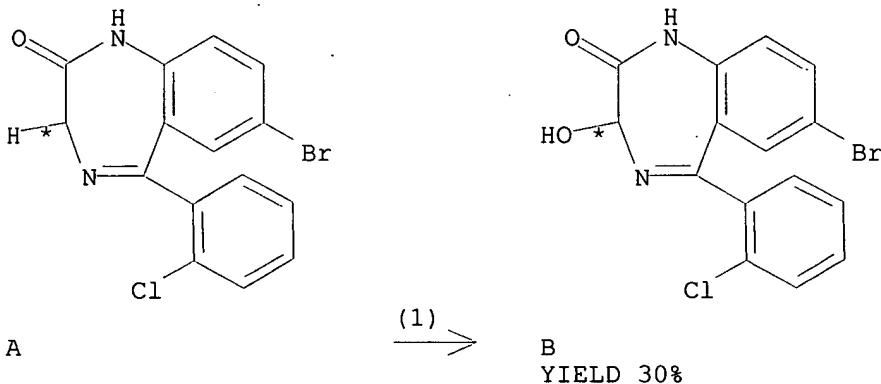
RX (2) OF 9      2 A ==> D + E...



RX(2) RCT A 604-75-1  
 RGT F 7789-20-0 D20  
 PRO D 95926-86-6, E 95926-87-7  
 SOL 75-05-8 MeCN

L61 ANSWER 15 OF 24 CASREACT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 102:147424 CASREACT  
 TITLE: Hydroxylation of 1,4-benzodiazepin-2-ones by actinomycetes  
 AUTHOR(S): Davidenko, T. I.; Zabolotskaya, N. N.; Milienko, N. P.; Andronati, S. A.; Kuznetsov, V. D.; Bogatskii, A. V.  
 CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, USSR  
 SOURCE: Doklady Akademii Nauk SSSR (1984), 278(4), 878-81  
 [Chem.]  
 CODEN: DANKAS; ISSN: 0002-3264  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Twenty-four strains of actinomycetes were able to transform 6 title compds. to the corresponding 3-hydroxy-1,4-benzodiazepin-2-ones. The highest rate of hydroxylation was obsd. with *Actinomyces roseochromogenes*, *A. lavendulae*, and *Streptomyces viridis*. The yield of 3-hydroxy derivs. was 30-40%. When the actinomycetes were immobilized in various carriers, esp. carrageenan [9000-07-1], 65% of the hydroxylation activity was retained. The 3-hydroxy derivs. are used as tranquilizers.

RX(1) OF 12 A ==> B

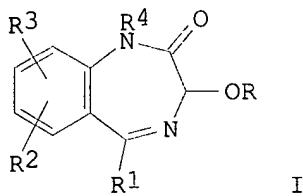


RX(1) RCT A 51753-57-2  
 PRO B 70030-11-4

L61 ANSWER 16 OF 24 CASREACT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 100:51612 CASREACT  
 TITLE: 3-Hydroxybenzodiazepinones  
 INVENTOR(S): Hardtmann, Goetz Eduard; Repic, Oljan; Vogt, Susi  
 PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 10 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1

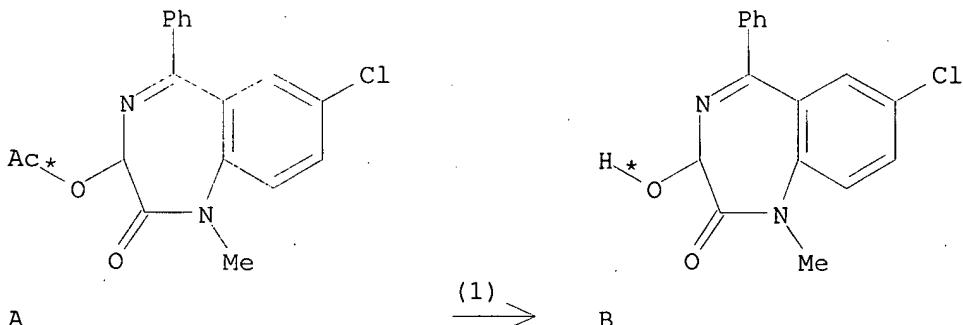
## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3314893	A1	19831103	DE 1983-3314893	19830425
US 4412952	A	19831101	US 1982-373450	19820430
FR 2526021	A1	19831104	FR 1983-6804	19830422
FR 2526021	B1	19870612		
CH 655930	A	19860530	CH 1983-2176	19830422
GB 2120245	A1	19831130	GB 1983-11446	19830427
GB 2120245	B2	19851023		
JP 58194865	A2	19831112	JP 1983-74194	19830428
CA 1195326	A1	19851015	CA 1983-426924	19830428
PRIORITY APPLN. INFO.:			US 1982-373450	19820430
GI				



AB Hydroxybenzodiazepinones I [R = H; R1 = (un)substituted Ph; R2, R3 = H, F3C, MeSO<sub>2</sub>, Br, Cl, NO<sub>2</sub>, R4 = alkyl] were prep'd. in high yield and purity by sapon. of I (R = acyl) with KOR5 (R5 = H, alkyl) in alc. Thus, I (R = Ac, R1 = Ph, R2 = 7-Cl, R3 = H, R4 = Me) was refluxed in MeOH with KOH to give, after crystn. from EtOH, 82.9% I (R = H, R1 = Ph, R2 = 7-Cl, R4 = Me) of 99.8% purity.

RX(1) OF 1      A    ==>    B



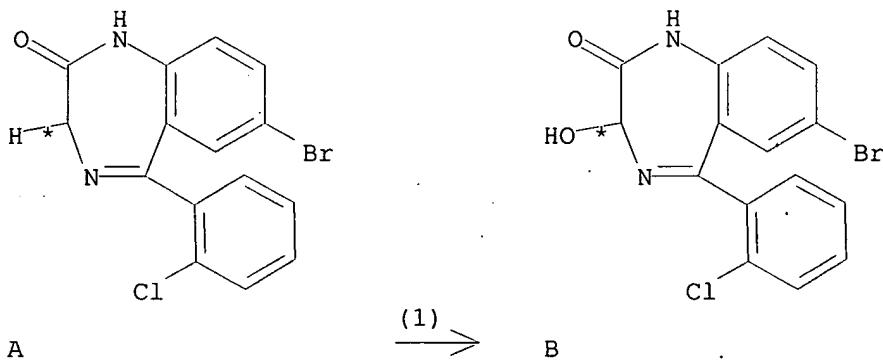
RX(1)      RCT    A 18818-64-9  
PRO    B 846-50-4

L61 ANSWER 17 OF 24    CASREACT    COPYRIGHT 2003 ACS  
ACCESSION NUMBER:    96:160848    CASREACT  
TITLE:    3-Hydroxy-7-bromo-5-(o-, m-, p-chloro)  
phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one and  
3-hydroxy-3-methyl-7-bromo-5-(o-, m-, p-chloro)  
phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one by  
fermentation

INVENTOR(S): Bogatskii, A. V.; Kuznetsov, V. D.; Davidenko, T. I.;  
Zabolotskaya, N. N.; Sereda, N. P.; Andronati, S. A.;  
Yakubovskaya, L. N.  
PATENT ASSIGNEE(S): Institute of Physical Chemistry, Academy of Sciences,  
Ukrainian S.S.R., USSR; Institute of Microbiology  
U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,  
Tovarnye Znaki 1981, (45), 144.  
SOURCE: CODEN: URXXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Russian  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

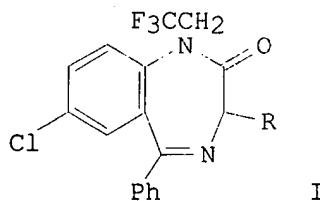
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 887625	A1	19811207	SU 1980-2928358	19800208
PRIORITY APPLN. INFO.:			SU 1980-2928358	19800208
AB	The title compds. are obtained by cultivating <i>Streptoverticillium cinnamoneum</i> VKM A-609 or <i>Streptomyces viridis</i> VKM A-607 in a nutrient medium contg. corn ext. 1.0, glucose 0.5, NaCl 0.5, (NH4)2SO4 0.3, CaCO3 0.5 and starch 1.5 g/100 g H2O at pH 6.8-7.0, adding (3-12 mg/100 mg medium) 7-bromo-5-(o-, m-, or p-chloro)phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one, incubating for 2-5 days at 28.degree., sepg. the products by extn. with CHCl3, EtOAc, petroleum ether, or a mixt. of C2H4Cl2 and EtOAc, and purifying by recrystn. from alc. or by column chromatog. on Al2O3, eluting with a mixt. of MeOH or EtOH and HOAc.			

RX(1) OF 1                    A ==> B



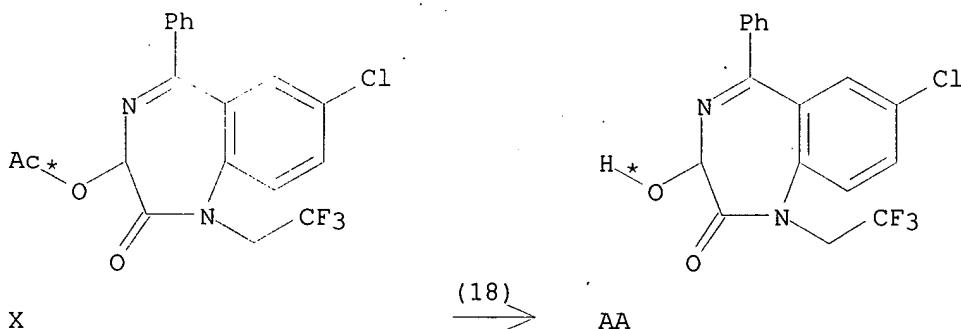
RX(1) RCT A 51753-57-2  
PRO B 70030-11-4

L61 ANSWER 18 OF 24    CASREACT    COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 94:121481    CASREACT  
TITLE: New synthesis of 2-(2',2',2'-trifluoroethyl)-amino-5-chlorobenzophenone and related studies  
AUTHOR(S): Oklobdzija, Milan; Fajdiga, Tatjana; Kovac, Tomislav; Zonno, Franco; Sega, Alessandro; Sunjic, Vitomir  
CORPORATE SOURCE: Chem. Res. Co., San Giovanni al Natisone, Italy  
SOURCE: Acta Pharmaceutica Jugoslavica (1980), 30(3), 121-33  
DOCUMENT TYPE: CODEN: APJUA8; ISSN: 0001-6667  
LANGUAGE: Journal  
GI: English



AB The haloazepam (I, R = H) intermediate 2,4-BzClC6H3NHCH2CF3 (II) was prep'd. by trifluoroacetyating 2,4-BzClC6H3NH2, redn. of 2,4-BzClC6H3NHCOCF3 with NaAlH2Et2, and oxidn. of 2,4-HOCHPhC1C6H3NHCH2CF3 with pyridinium dichromate. II was also obtained by treating 2,4-BzClC6H3NH2 with CF3CO2H-NaBH4. Acylation of II with BrCH2COBr and ring closure with hexamine gave I (R = H) which was acetoxylated and treated with NaOMe to give I (R = OH). Reductive trifluoroethylation of demethyldiazepam occurred in the 4-position only.

RX(18) OF 53 ...X ==> AA



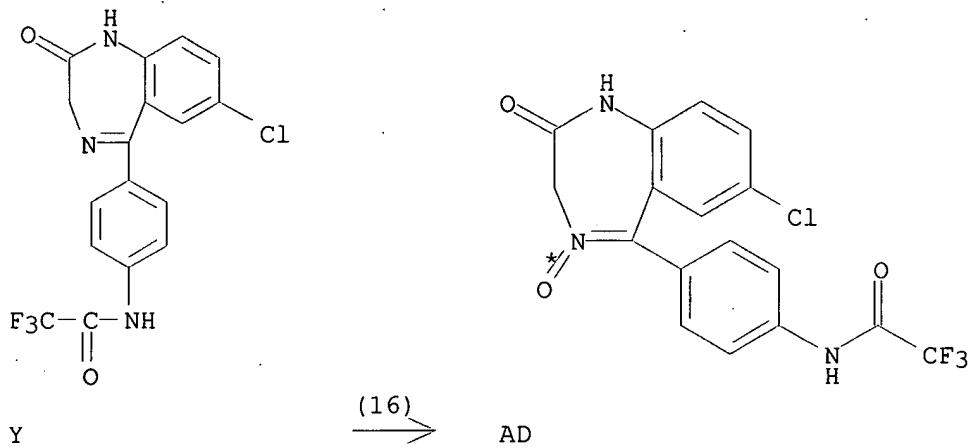
RX(18) RCT X 22753-74-8  
PRO AA 22753-75-9  
CAT 124-41-4 NaOMe

L61 ANSWER 19 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 92:41904 CASREACT  
TITLE: Quinazolines and 1,4-benzodiazepines. LXXXIX:  
Haptens useful in benzodiazepine immunoassay  
development  
AUTHOR(S): Earley, James V.; Fryer, R. Ian; Ning, Robert Y.  
CORPORATE SOURCE: Dep. Chem. Res., Hoffmann-La Roche Inc., Nutley, NJ,  
07110, USA  
SOURCE: Journal of Pharmaceutical Sciences (1979); 68(7),  
845-50  
CODEN: JPMSAE; ISSN: 0022-3549  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

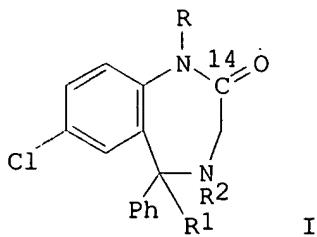
AB Benzodiazepines I (R = H, Me; R1 = H, AcO, HO; R2 = HO, F3CCONH, MeO2CCH2O, MeO, H2NCOCH2O, H2NNHCOCH2O, H2N; R3 = H, H2NC6H4N:N; n = 1, 0), II (R4 = HO, H2N, MeO2CCH2O, H2NNHCOCH2O, H2NCH2CH2CH2O), and III (R5 = H, HO2CCH2CH2O; R6 = HN, NO2; R7 = H, Cl) were prep'd. as haptens for use in immunoassay anal. Thus, cyclocondensation of the benzophenone IV in NH3(1) gave 67% I (R = R1 = R3 = H; R2 = HO; n = 0), and treatment of quinazoline V with MeNH2 in MeOH gave II (R4 = HO).

RX(16) OF 123 ...Y ==> AD...



RX(16) RCT Y 67445-91-4  
 PRO AD 67445-92-5  
 CAT 937-14-4 MCPBA

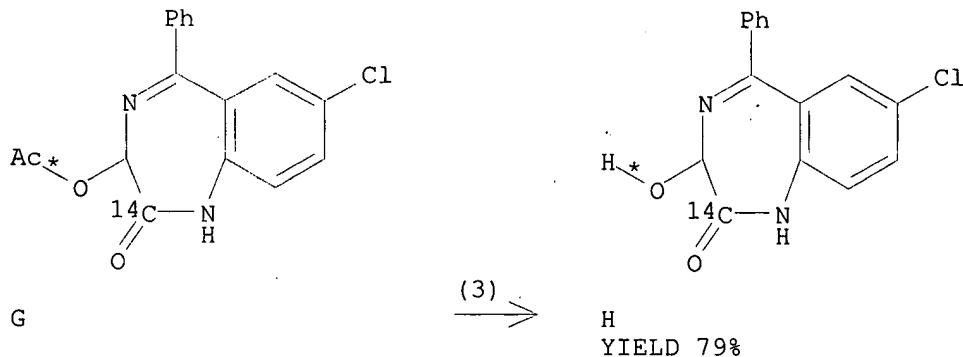
L61 ANSWER 20 OF 24 CASREACT COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 92:22479 CASREACT  
 TITLE: Synthesis of 2-14C-labeled 3H-1,4-benzodiazepines  
 AUTHOR(S): Tegyey, Zsuzsanna; Maksay, G.; Otvos, L.  
 CORPORATE SOURCE: Cent. Res. Inst. Chem., Budapest, Hung.  
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals  
 (1979), 16(3), 377-85  
 CODEN: JLCRD4; ISSN: 0362-4803  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Di- and tetrahydrobenzodiazepinones I (R = H, R1R2 = bond; R = Me, R1 = H, R2 = H, CONH2) were prep'd. (radiochem. yield 28.9, 9.5 and 25.3%, resp.)

in 5, 3 and 4 steps, resp., from  $\text{PhCH}_2\text{O}_2\text{CNHCH}_2\text{I}_4\text{COCl}$  and  $4,2\text{-Cl}(\text{PhCO})\text{C}_6\text{H}_3\text{NHR}$ .

RX(3) OF 14 ...G ==> H



RX(3) RCT G 72216-21-8  
PRO H 3855-66-1

L61 ANSWER 21 OF 24 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER:

91:157698 CASREACT

TITLE:

1,4-Benzodiazepines and their cyclic homologs and analogs. 30. Synthesis and properties of 3- and 7-amino-5-phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-ones

AUTHOR(S):

Zhilina, Z. I.; Bogatskii, A. V.; Andronati, S. A.; Danilina, N. I.

CORPORATE SOURCE:

Fiz.-Khim. Inst., Odessa, 270080, USSR

SOURCE:

Khimiya Geterotsiklicheskikh Soedinenii (1979), (4), 545-9

DOCUMENT TYPE:

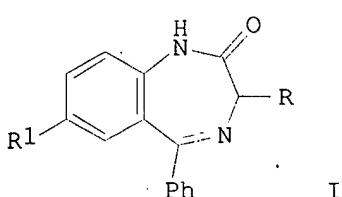
CODEN: KGSSAQ; ISSN: 0453-8234

LANGUAGE:

Journal

GI

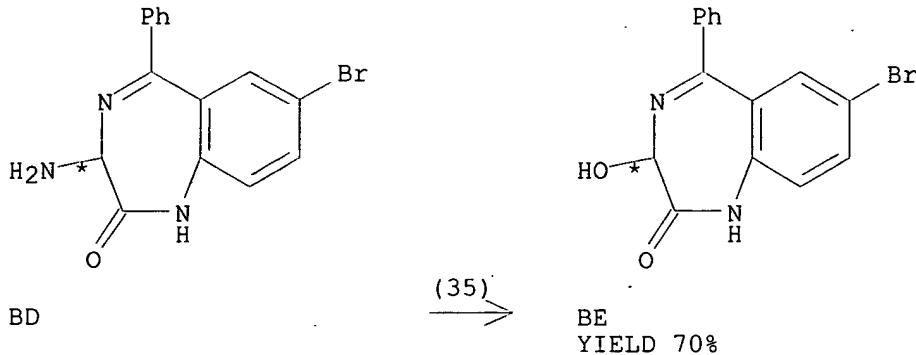
Russian



AB The 3-aminobenzodiazepinones I ( $R = \text{NH}_2$ ;  $R1 = \text{H, Me, Br, Cl}$ ) (II) were prep'd. from  $2,4-(\text{Bz})\text{R1C}_6\text{H}_3\text{NHCOCH}_2\text{Cl}$  by iodination to give  $2,4-(\text{Bz})\text{R1C}_6\text{H}_3\text{NHCOCH}_2\text{I}$ , which underwent hydroxyamination to give  $2,4-(\text{Bz})\text{R1C}_6\text{H}_3\text{NHCOCH}_2\text{NHOH}$ ; treatment of the latter with  $\text{Ac}_2\text{O}$  and then cyclocondensation in  $\text{EtOH}$  contg.  $\text{NH}_3$  and hydrolysis gave II. 7-Aminobenzodiazepinone I ( $R = \text{H}$ ;  $R1 = \text{NH}_2$ ) (III) was prep'd. by redn. of I ( $R1 = \text{NO}_2$ ). II and III formed Schiff bases on condensation with benzaldehydes in aprotic solvents contg. acid catalysts, e.g.  $\text{ZnCl}_2$ . Treatment of I ( $R = \text{AcNH}$ ;  $R1 = \text{Cl}$ ) with  $\text{P}_2\text{S}_5$  gave I [ $R = \text{MeC}(\text{S})\text{NH}$ ;  $R1 = \text{Cl}$ ], and diazotization-hydrolysis of I ( $R = \text{NH}_2$ ;  $R1 = \text{Br}$ ) gave I ( $R = \text{HO}$ ).

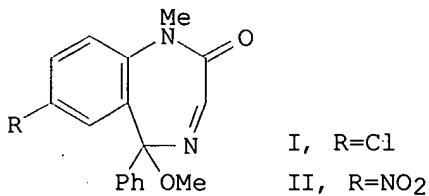
Polarog. redn. curves of the Schiff bases of II were detd.

RX(35) OF 146 . . . . BD ==> BE



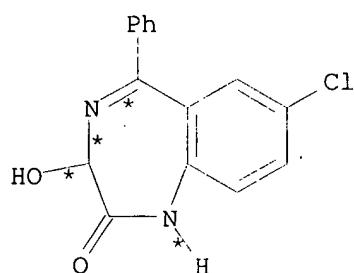
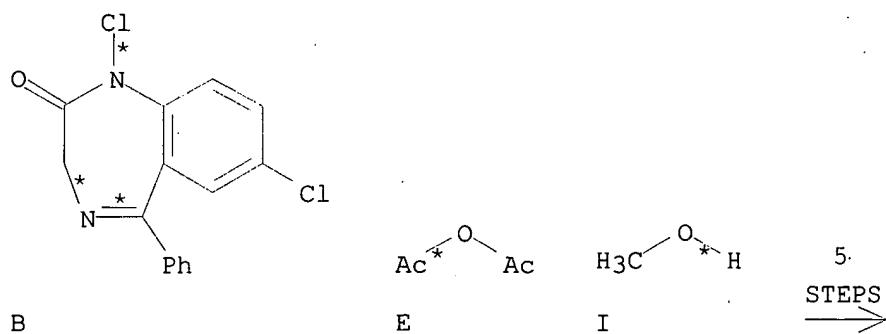
RX(35) RCT BD 70890-49-2  
RGT BF 7782-77-6 HNO<sub>2</sub>  
PRO BE 37891-18-2

L61 ANSWER 22 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 87:33437 CASREACT  
TITLE: 5-Aryl-1,5-dihydro-2H-1,4-benzodiazepin-2-one derivatives as antianxiety agents  
AUTHOR(S): Ogata, Masaru; Matsumoto, Hiroshi; Hirose, Katsumi  
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan  
SOURCE: Journal of Medicinal Chemistry (1977), 20(6), 776-81  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB A series of 18 7-chloro- or 7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one derivs. were prep'd. and tested in mice for acute toxicity and activity as muscle relaxants, tranquilizers, and anticonvulsants. 7-Chloro-1,5-dihydro-5-methoxy-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one (I) [62658-15-5] and 1,5-dihydro-5-methoxy-1-methyl-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one (II) [62159-90-4] had activity comparable to or greater than diazepam [439-14-5]. Structure-activity relations are discussed.

RX(93) OF 101 COMPOSED OF RX(8), RX(9), RX(12), RX(15), RX(6)  
RX(93) B + E + I ==> Q



Q  
YIELD 81%

RX(8) RCT B 10378-81-1, E 108-24-7  
RGT G 7697-37-2 HNO3  
PRO T 62658-06-4

RX(9) RCT T 62658-06-4  
PRO U 62658-09-7  
CAT 74-89-5 MeNH2

RX(12) RCT U 62658-09-7, I 67-56-1  
PRO N 62159-89-1  
SOL 67-56-1 MeOH

RX(15) RCT N 62159-89-1  
PRO K 61983-99-1  
CAT 121-44-8 Et3N

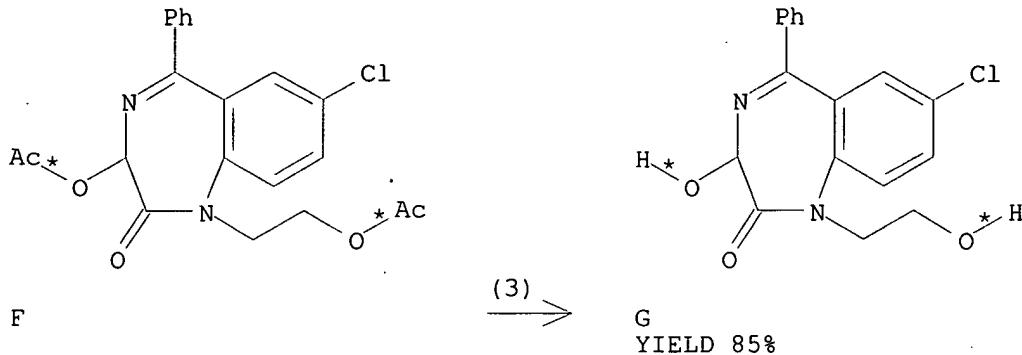
RX(6) RCT K 61983-99-1  
PRO Q 604-75-1

L61 ANSWER 23 OF 24 CASREACT COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 83:164140 CASREACT  
TITLE: New series of benzodiazepines. 1-Hydroxyalkyl derivatives of 1,3-dihydro-2H-1,4-benzodiazepin-2-ones  
AUTHOR(S): Tamagnone, G. F.; De Maria, R.; De Marchi, F.  
CORPORATE SOURCE: Res. Dep., Schiapparelli S.p.A., Turin, Italy  
SOURCE: Arzneimittel-Forschung (1975), 25(5), 720-2  
CODEN: ARZNAD; ISSN: 0004-4172  
DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Twenty-four potential hypnotics I [R = OH, O<sub>2</sub>C(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>H, OAc, Cl, NEt<sub>2</sub>; R<sub>1</sub> = H, OAc, OH, OEt; R<sub>2</sub> = H, Cl, F; R<sub>3</sub> = Cl, NO<sub>2</sub>, n = 2, 3] or their oxides were prepd. by 1-alkylating the appropriate phenylbenzodiazepinones and usual reactions (acylation, hydrolysis, etc.).

RX(3) OF 22      F    ==>    G...



RX(3)      RCT F 56875-82-2  
 RGT H 7664-41-7 NH3  
 PRO G 51230-34-3

L61 ANSWER 24 OF 24 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 74:31735 CASREACT

TITLE: Nitrone isomerization in the 1,4-benzodiazepine series

AUTHOR(S): Schlagler, Ludwig H.

CORPORATE SOURCE: Gerot Pharm., Vienna, Austria

SOURCE: Tetrahedron Letters (1970), (51), 4519-20

CODEN: TELEAY; ISSN: 0040-4039

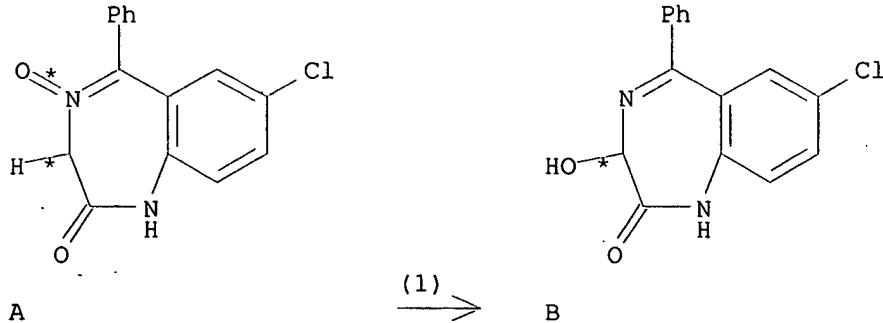
DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The nitrone (I) is converted to oxazepam (II) in a 1-step reaction by treatment with a Lewis acid in the presence of a nitrile, such as MeCN or acrylonitrile. I is treated with BF<sub>3</sub> to give an adduct which is kept in the nitrile at room temp. to give II. II is obtained from I without adduct formation when AlCl<sub>3</sub> is used.

RX(1) OF 1      A    ==>    B



RX(1) RCT A **963-39-3**  
RGT C 7446-70-0 AlCl3  
PRO B **604-75-1**  
SOL 109-99-9 THF, 75-05-8 MeCN  
NTE Classification: N-Deoxygenation; Hydroxylation; Migration; #  
Conditions: AlCl3; THF; MeCN; 20 deg; # Comments: acrylonitrile  
can also be used as solvent, BF3.Et2O as alternative reagent

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